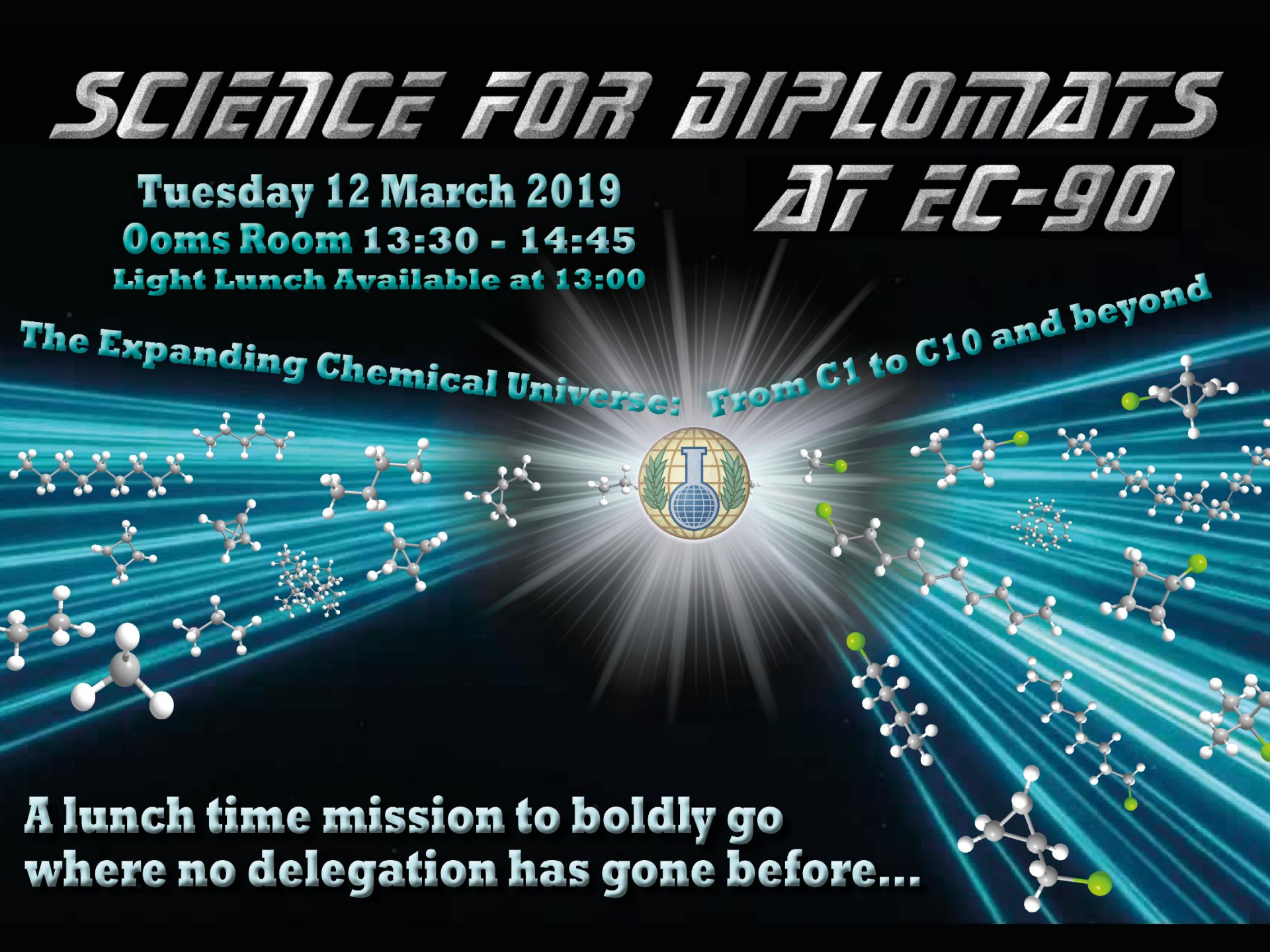
SCIENCE FOR DIPLOMATS AT EC-90

Tuesday 12 March 2019
Ooms Room 13:30 - 14:45
Light Lunch Available at 13:00

The Expanding Chemical Universe: From C1 to C10 and beyond



A lunch time mission to boldly go where no delegation has gone before…

OPCW

Organisation for the Prohibition of Chemical Weapons

The Expanding Chemical Universe: From C1 to C10 and Beyond

Science for Diplomats at EC-90

The Hague, 12 March 2019

Starring:

Mr Cheng Tang, SAB Chair

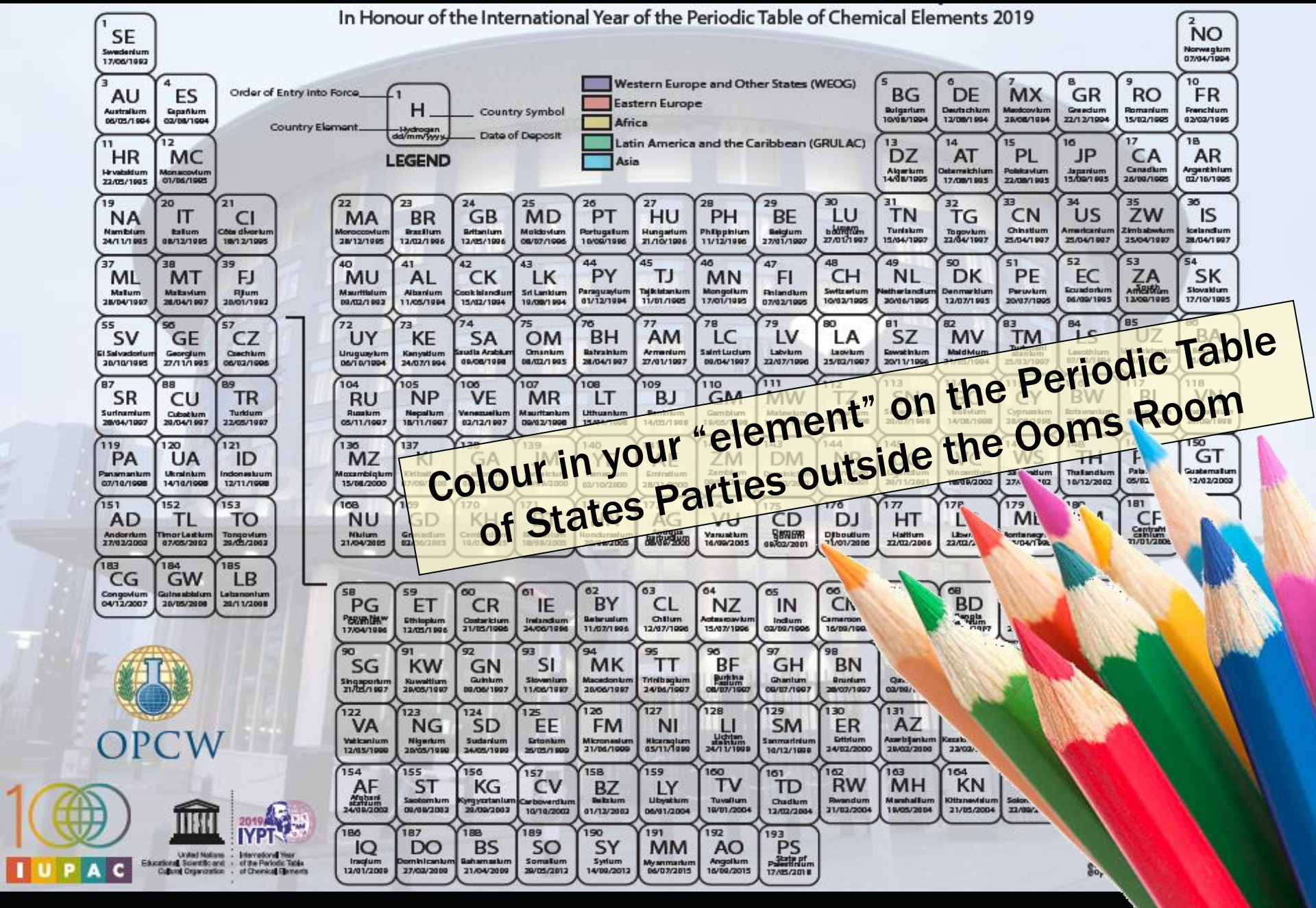
Dr Jonathan E. Forman, Science Policy Adviser and SAB Secretary

Mr Peter Brud, Ms Maria Hemme, and Ms Giovanna Pontes

Office of Strategy and Policy

With special guest star Ms Andrea Dymytrova

Let us Know You are Here!



Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Schedule 1

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:

(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:

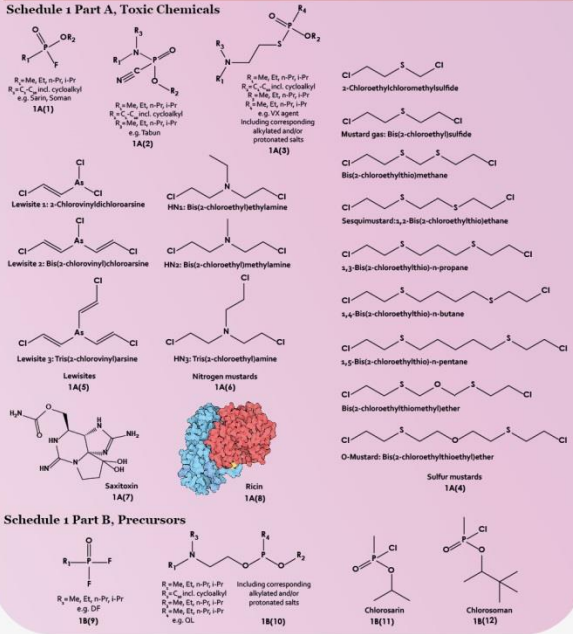
(i) It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparableproperties;

(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 1 Part A, Toxic Chemicals



Schedule 1 Part B, Precursors

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:

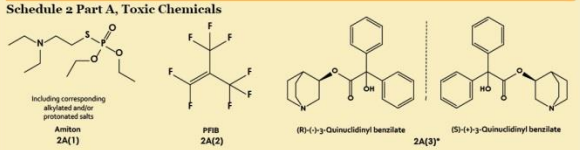
(a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;

(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;

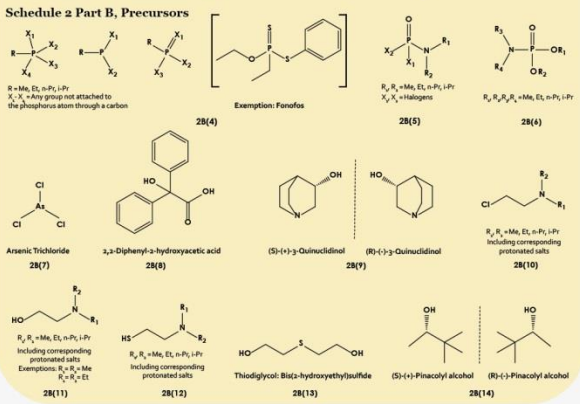
(c) It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;

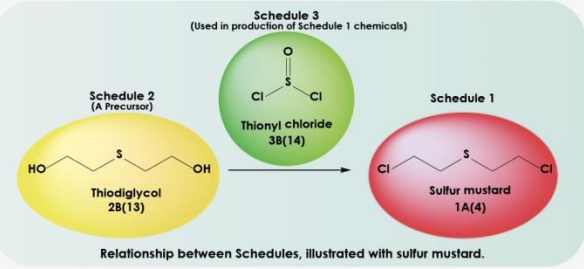
(d) It is not produced in large commercial quantities for purposes not prohibited under this Convention.

Schedule 2 Part A, Toxic Chemicals



Schedule 2 Part B, Precursors





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:

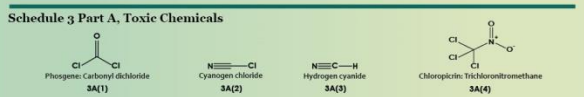
(a) It has been produced, stockpiled or used as a chemical weapon;

(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;

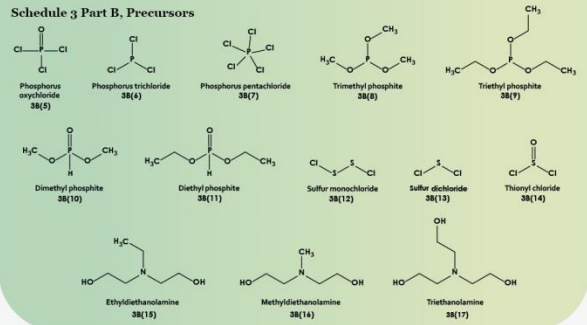
(c) It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, part B;

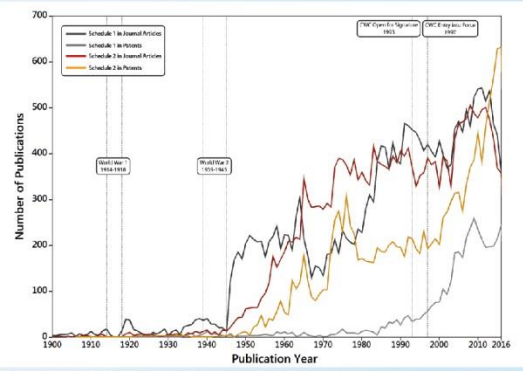
(d) It may be produced in large commercial quantities for purposes not prohibited under this Convention.

Schedule 3 Part A, Toxic Chemicals



Schedule 3 Part B, Precursors





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.

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

@opcw @opcw_st /opcwonline /opcwonline /company/opcw /opcw

Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Scientific Advisory Board's Recommendations to the Fourth Review Conference of the Chemical Weapons Convention

A quick reference guide to the executive summary recommendations of the OPCW Scientific Advisory Board's report on developments in science and technology to the Fourth Review Conference (RC-4/DG.1, dated 30 April 2018).

Download RC-4/DG.1

PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

@opcw @opcw_st /opcwonline /opcwonline /company/opcw /opcw

Schedule 2

Schedule 2

taken into account in considering whether a toxic
1 or a precursor to a Schedule 1 chemical or to a
rt A, should be included in Schedule 2:
o the object and purpose of this Convention because
r incapacitating toxicity as well as other properties
used as a chemical weapon;

Thiodiglycol: Bis(2-hydroxyethyl)sulfide
2B(13)

(S)-(+)-Pinacolyl alcohol
2B(14)

(R)-(-)-Pinacolyl alcohol

Schedule 3
production of Schedule 1 chemicals)

Thionyl chloride
3B(14)

Thiodiglycol
2B(13)

Schedule 1

Sulfur mustard
1A(4)

Relationship between Schedules, illustrated with sulfur mustard.

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:

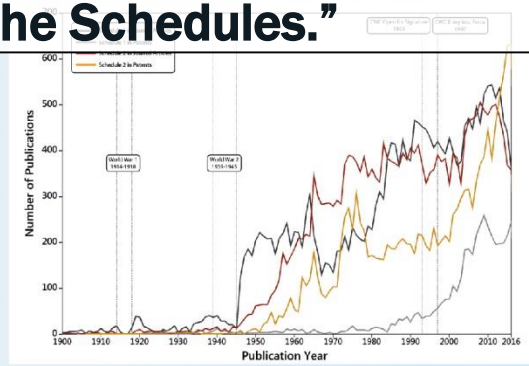
(a) It has been produced, stockpiled or used as a chemical weapon;

possesses such lethal or incapacitating toxicity as well as other properties that

importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, Part B;

Schedule 3 Part A. Toxic Chemicals:

> **"Given the substantial changes in chemistry and chemical industry since the schedules were finalised a quarter century ago, a review of the schedules should be considered to assess whether: (a) the chemicals currently listed are in the appropriate Schedule, and (b) any toxic chemicals or specific precursors should be added to or removed from the Schedules."**



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.

Scheduled Chemicals under the Chemical Weapons Convention (CWC)

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:

- been produced, stockpiled or used as a chemical weapon;
- such lethal or incapacitating toxicity as well as other properties that
- in the production of one or more chemicals listed in Schedule 1 or

ntial changes in
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OPCW

Technical Secretariat

S/1682/2018
25 October 2018
Original: ENGLISH

NOTE BY THE DIRECTOR-GENERAL

JOINT PROPOSAL BY CANADA, THE NETHERLANDS, AND THE UNITED STATES OF AMERICA FOR A TECHNICAL CHANGE TO SCHEDULE 1 OF THE ANNEX ON CHEMICALS TO THE CHEMICAL WEAPONS CONVENTION

1. The Director-General has received a joint proposal from Canada, the Netherlands, and the United States of America for a technical change to Schedule 1 of the Annex on Chemicals to the Chemical Weapons Convention (hereinafter "the Convention").

2. Pursuant to paragraphs 4 and 5 of Article XV of the Convention, the Director-General hereby communicates information regarding the above-mentioned proposals, which were received on proposed text can be found in the Attachment to this Note. The Russian Federation's highly protected "Technical Change Proposal" dated 25 October 2018). Accordingly, these proposals will be evaluated by the Technical the Chemical Weapons Convention Secretariat and are subject to different timelines under paragraph 5 of Article XV of the 16 October 2018 via note verbale, is available for consultation at the Convention.
OPCW Headquarters.

Attachment: United States, Canada, and the Netherlands: Joint Proposal for Additions to Schedule 1 of the Annex on Chemicals to the Chemical Weapons Convention

CS-2018-1422(E) distributed 25/10/2018

OPCW

Technical Secretariat

S/1697/2018
7 December 2018
Original: ENGLISH

NOTE BY THE DIRECTOR-GENERAL

PROPOSALS TO INTRODUCE ADDITIONS TO THE SCHEDULES OF CHEMICALS OF THE ANNEX ON CHEMICALS TO THE CONVENTION ON THE PROHIBITION OF THE DEVELOPMENT, PRODUCTION, STOCKPILING AND USE OF CHEMICAL WEAPONS AND ON THEIR DESTRUCTION

1. The Director-General has received a note verbale from the Russian Federation submitting proposals to introduce additional families to the schedules of chemicals contained in the Annex on Chemicals to the Convention on the Prohibition of the Development, Production, Stockpiling, and Use of Chemical Weapons and on their Destruction (hereinafter "the Convention").

2. Pursuant to paragraphs 4 and 5 of Article XV of the Convention, the Director-General hereby communicates the above-mentioned proposals, which were received on 30 November 2018. The proposed text can be found in the Attachment to this Note.

3. The Russian Federation's proposals will be considered as a second and separate set of proposals from the joint proposal from Canada, the Netherlands, and the United States of America for a technical change to Schedule 1 of the Annex on Chemicals S/1682/2018, dated 25 October 2018). Accordingly, these proposals will be evaluated by the Technical Secretariat and are subject to different timelines under paragraph 5 of Article XV of the Convention.

4. The Russian Federation submitted additional information through Note Verbale 2295, dated 21 November 2018 (RC-4/NAT.35, dated 5 December 2018) for consideration with respect to its proposals as well as to the joint proposal.

5. In accordance with subparagraph 5(a) of Article XV of the Convention, the proposals submitted by the Russian Federation are being transmitted to the Depositary.

Attachment: Note Verbale from the Russian Federation dated 29 November 2018

CS-2018-1621(E) distributed 07/12/2018

Scientific Advisory Board to the Fourth Review Conference

A quick reference guide to the executive summary of the OPCW Scientific Advisory Board's report on developments in science and technology to the Fourth Review Conference

Download RC-4/DG.1

PROHIBITION OF CHEMICAL WEAPONS
Working Together for a World Free of Chemical Weapons

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Thiodiglycol 2B(13)

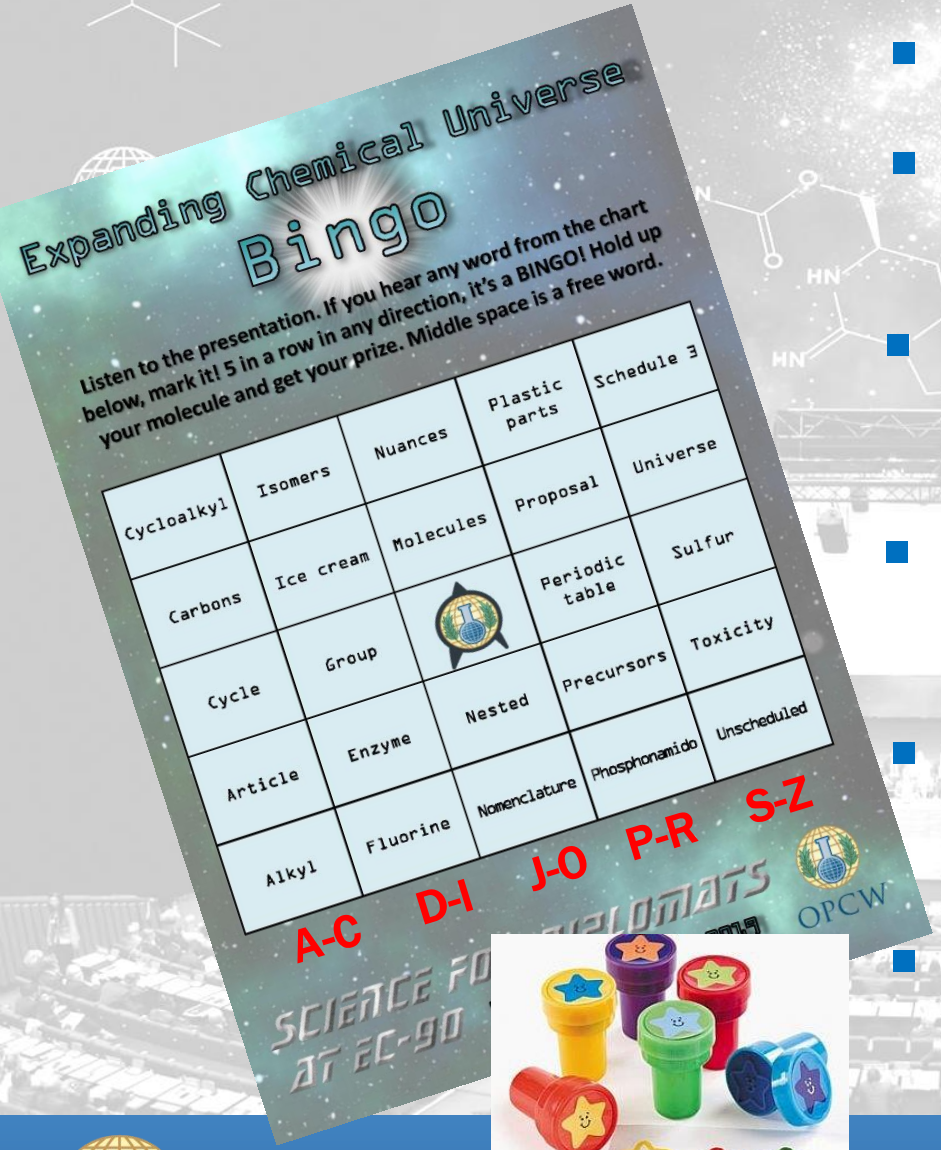
Relationship between Schedules, illust

Publication Year

1960 1970 1980 1990 2000 2010 2016

...hose in schedules 1 and 2, can have scientifically and economically ...captures the number of yearly scientific publications that refer to them.

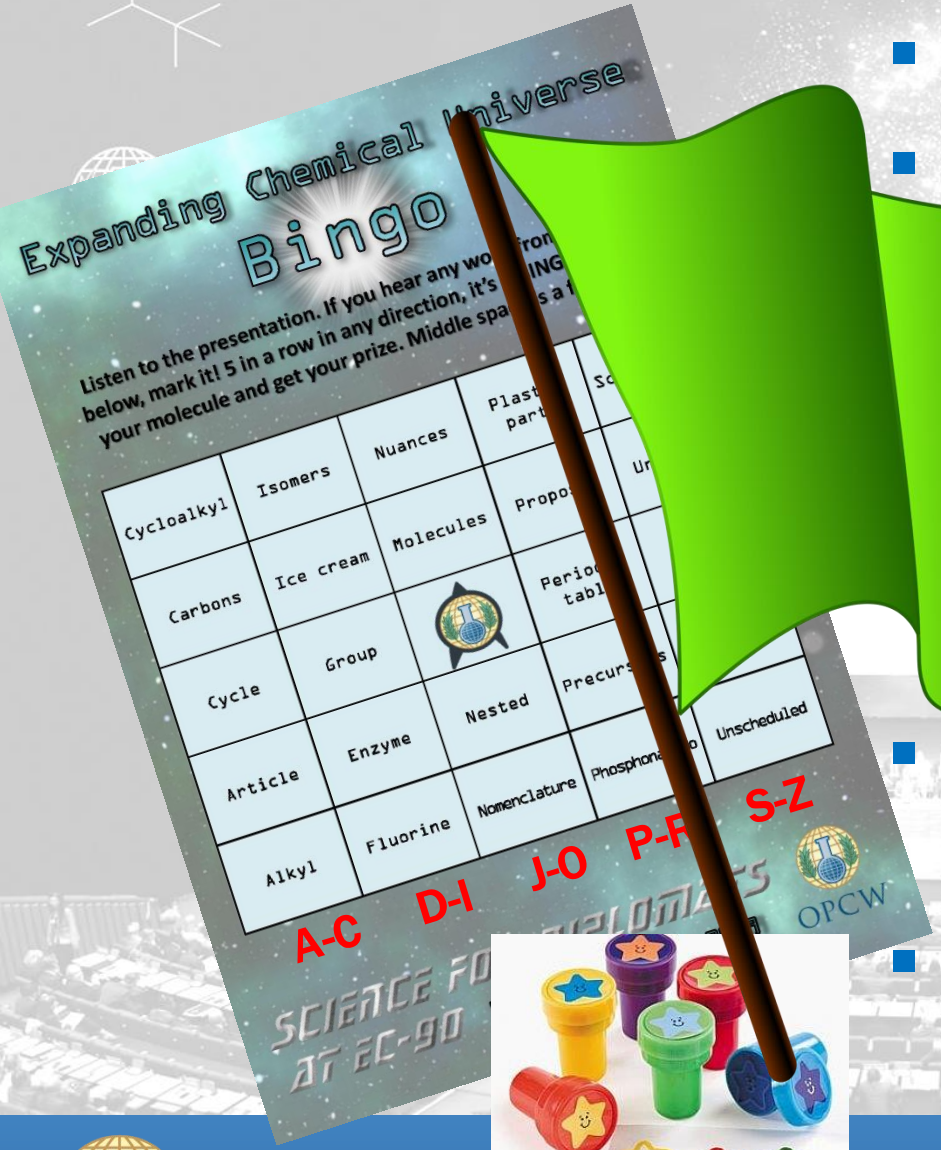
Before We Begin…



- Listen to the Science Adviser
- ***Stamp words as you hear them!***
- A stamped horizontal, vertical or diagonal row of 5 "wins"
- **1st person to get a Bingo wins "acetylcholinesterase"**
- Next prizes are "Schedule 1" Key Chains
- After 1st Bingo, 1st Bingo in a chair wins a model kit

OPCW

Before We Begin…



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- d horizontal, vertical
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  cholinesterase"
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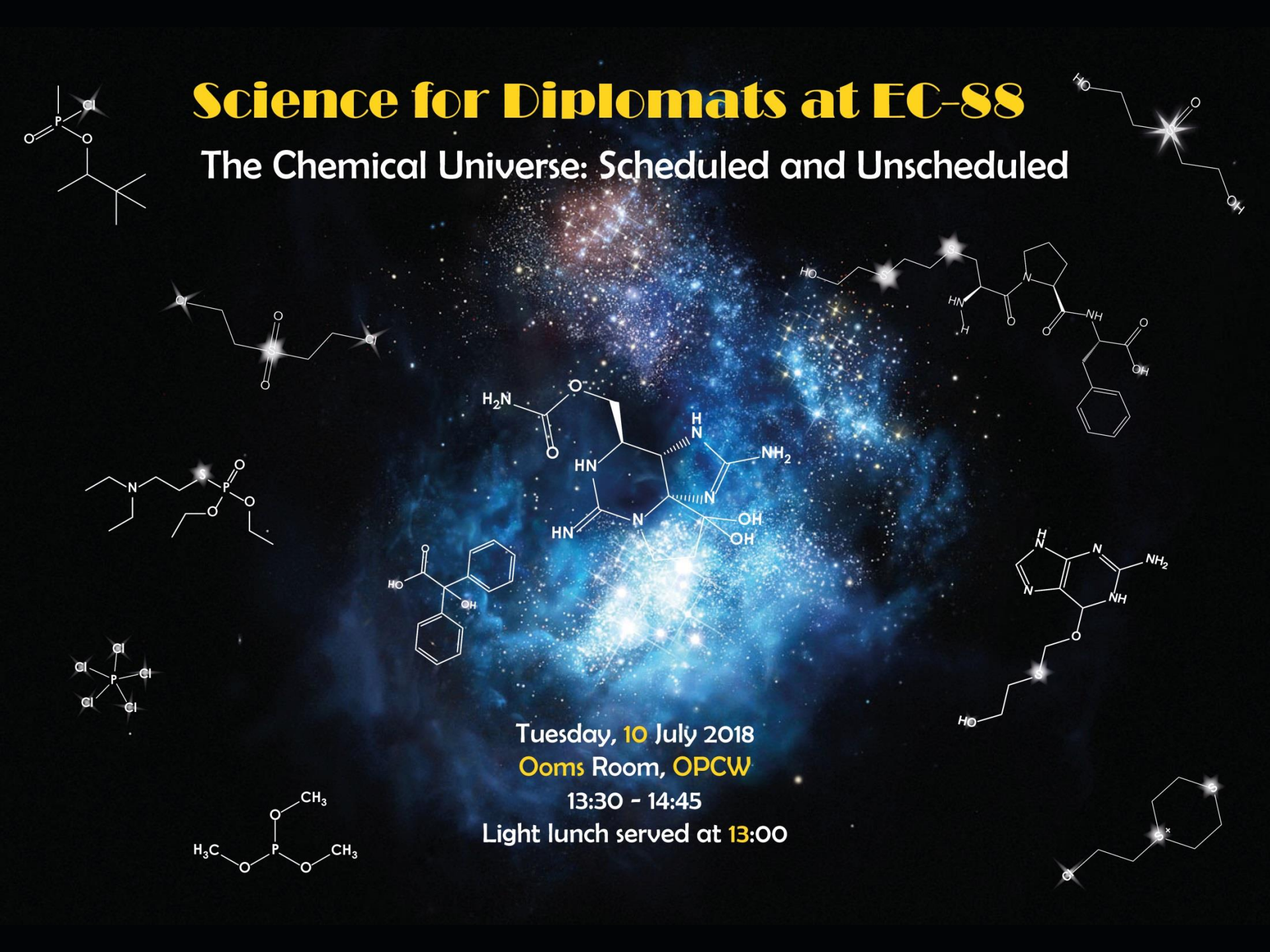
OPCW

Science for Diplomats at EC-88

The Chemical Universe: Scheduled and Unscheduled



Tuesday, 10 July 2018

Ooms Room, OPCW

13:30 - 14:45

Light lunch served at 13:00

B. SCHEDULES OF CHEMICALS

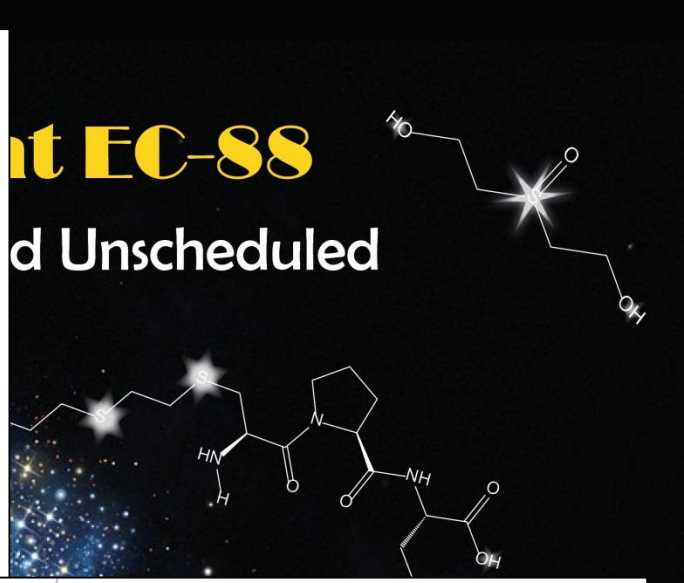
The following Schedules list toxic chemicals and their precursors. For the purpose of implementing this Convention, these Schedules identify chemicals for the application of verification measures according to the provisions of the Verification Annex. Pursuant to Article II, subparagraph 1 (a), these Schedules do not constitute a definition of chemical weapons.

(Whenever reference is made to groups of dialkylated chemicals, followed by a list of alkyl groups in parentheses, all chemicals possible by all possible combinations of alkyl groups listed in the parentheses are considered as listed in the respective Schedule as long as they are not explicitly exempted. A chemical marked "*" on Schedule 2, part A, is subject to special thresholds for declaration and verification, as specified in Part VII of the Verification Annex.)

Schedule 1

		(CAS registry number)
A.	Toxic chemicals:	
(1)	O-Alkyl ($\leq C_{10}$, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates	
	e.g. Sarin: O-Isopropyl methylphosphonofluoridate	(107-44-8)
	Soman: O-Pinacolyl methylphosphonofluoridate	(96-64-0)
(2)	O-Alkyl ($\leq C_{10}$, incl. cycloalkyl) N,N-dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidocyanidates	
	e.g. Tabun: O-Ethyl N,N-dimethyl phosphoramidocyanidate	(77-81-6)
(3)	O-Alkyl (H or $\leq C_{10}$, incl. cycloalkyl) S-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonothiolates and corresponding alkylated or protonated salts	
	e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate	(50782-69-9)
(4)	Sulfur mustards:	
	2-Chloroethylchloromethylsulfide	(2625-76-5)
	Mustard gas: Bis(2-chloroethyl)sulfide	(505-60-2)
	Bis(2-chloroethylthio)methane	(63869-13-6)
	Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane	(3563-36-8)
	1,3-Bis(2-chloroethylthio)-n-propane	(63905-10-2)
	1,4-Bis(2-chloroethylthio)-n-butane	(142868-93-7)
	1,5-Bis(2-chloroethylthio)-n-pentane	(142868-94-8)
	Bis(2-chloroethylthiomethyl)ether	(63918-90-1)
	O-Mustard: Bis(2-chloroethylthioethyl)ether	(63918-89-8)

(5)	Lewisites:	
	Lewisite 1: 2-Chlorovinyldichloroarsine	(541-25-3)
	Lewisite 2: Bis(2-chlorovinyl)chloroarsine	(40334-69-8)
	Lewisite 3: Tris(2-chlorovinyl)arsine	(40334-70-1)
(6)	Nitrogen mustards:	
	HN1: Bis(2-chloroethyl)ethylamine	(538-07-8)
	HN2: Bis(2-chloroethyl)methylamine	(51-75-2)
	HN3: Tris(2-chloroethyl)amine	(555-77-1)
(7)	Saxitoxin	(35523-89-8)
(8)	Ricin	(9009-86-3)
B.	Precursors:	
(9)	Alkyl (Me, Et, n-Pr or i-Pr) phosphonyldifluorides	
	e.g. DF: Methylphosphonyldifluoride	(676-99-3)
(10)	O-Alkyl (H or $\leq C_{10}$, incl. cycloalkyl) O-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonites and corresponding alkylated or protonated salts	
	e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite	(57856-11-8)
(11)	Chlorosarin: O-Isopropyl methylphosphonochloridate	(1445-76-7)
(12)	Chlorosoman: O-Pinacolyl methylphosphonochloridate	(7040-57-5)

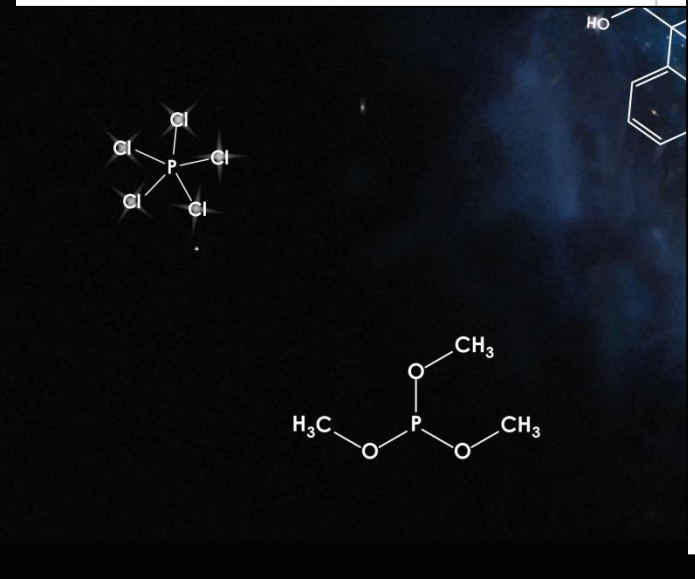


Schedule 2

A.	Toxic chemicals:	
(1)	Amiton: O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate and corresponding alkylated or protonated salts	(78-53-5)
(2)	PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene	(382-21-8)
(3)	BZ: 3-Quinuclidinyl benzilate (*)	(6581-06-2)
B.	Precursors:	
(4)	Chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms,	
	e.g. Methylphosphonyl dichloride	(676-97-1)
	Dimethyl methylphosphonate	(756-79-6)
	Exemption: Fonofos: O-Ethyl S-phenyl ethylphosphonothiolothionate	(944-22-9)
(5)	N,N-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides	
(6)	Dialkyl (Me, Et, n-Pr or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates	
(7)	Arsenic trichloride	(7784-34-1)
(8)	2,2-Diphenyl-2-hydroxyacetic acid	(76-93-7)
(9)	Quinuclidin-3-ol	(1619-34-7)
(10)	N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts	
(11)	N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-ols and corresponding protonated salts	
	Exemptions: N,N-Dimethylaminoethanol and corresponding protonated salts	(108-01-0)
	N,N-Diethylaminoethanol and corresponding protonated salts	(100-37-8)
(12)	N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-thiols and corresponding protonated salts	
(13)	Thiodiglycol: Bis(2-hydroxyethyl)sulfide	(111-48-8)
(14)	Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol	(464-07-3)

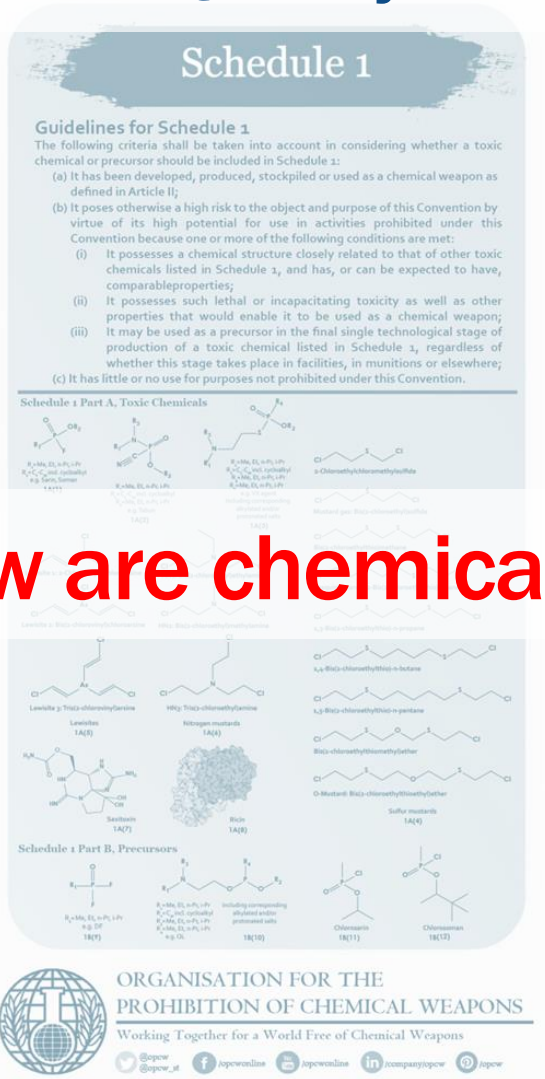
Schedule 3

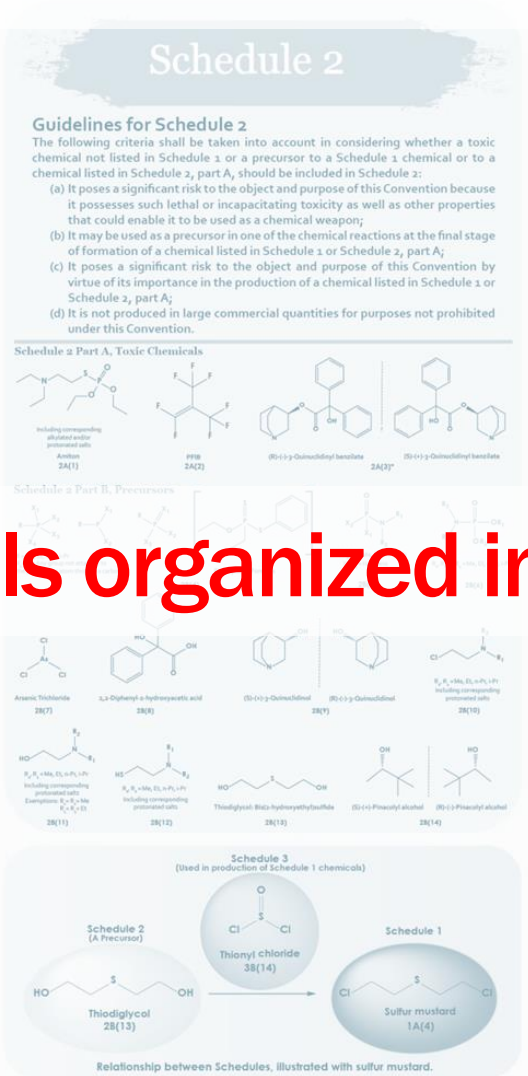
A.	Toxic chemicals:	
(1)	Phosgene: Carbonyl dichloride	(75-44-5)
(2)	Cyanogen chloride	(506-77-4)
(3)	Hydrogen cyanide	(74-90-8)
(4)	Chloropicrin: Trichloronitromethane	(76-06-2)
B.	Precursors:	
(5)	Phosphorus oxychloride	(10025-87-3)
(6)	Phosphorus trichloride	(7719-12-2)
(7)	Phosphorus pentachloride	(10026-13-8)
(8)	Trimethyl phosphite	(121-45-9)
(9)	Triethyl phosphite	(122-52-1)
(10)	Dimethyl phosphite	(868-85-9)
(11)	Diethyl phosphite	(762-04-9)
(12)	Sulfur monochloride	(10025-67-9)
(13)	Sulfur dichloride	(10545-99-0)
(14)	Thionyl chloride	(7719-09-7)
(15)	Ethyldiethanolamine	(139-87-7)
(16)	Methyldiethanolamine	(105-59-9)
(17)	Triethanolamine	(102-71-6)

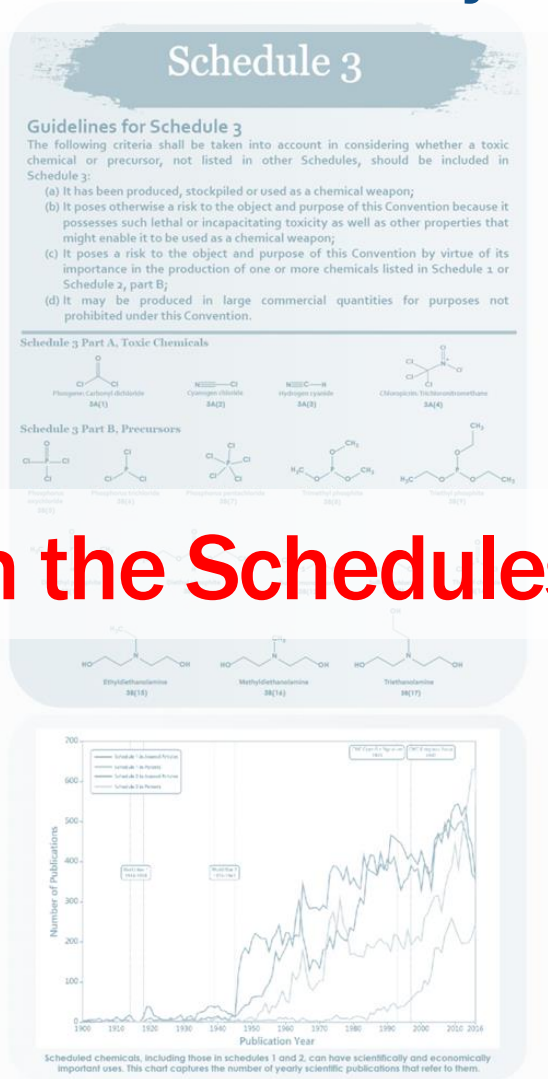


What Do You Remember?

Lets Quickly Review Where we left of from July

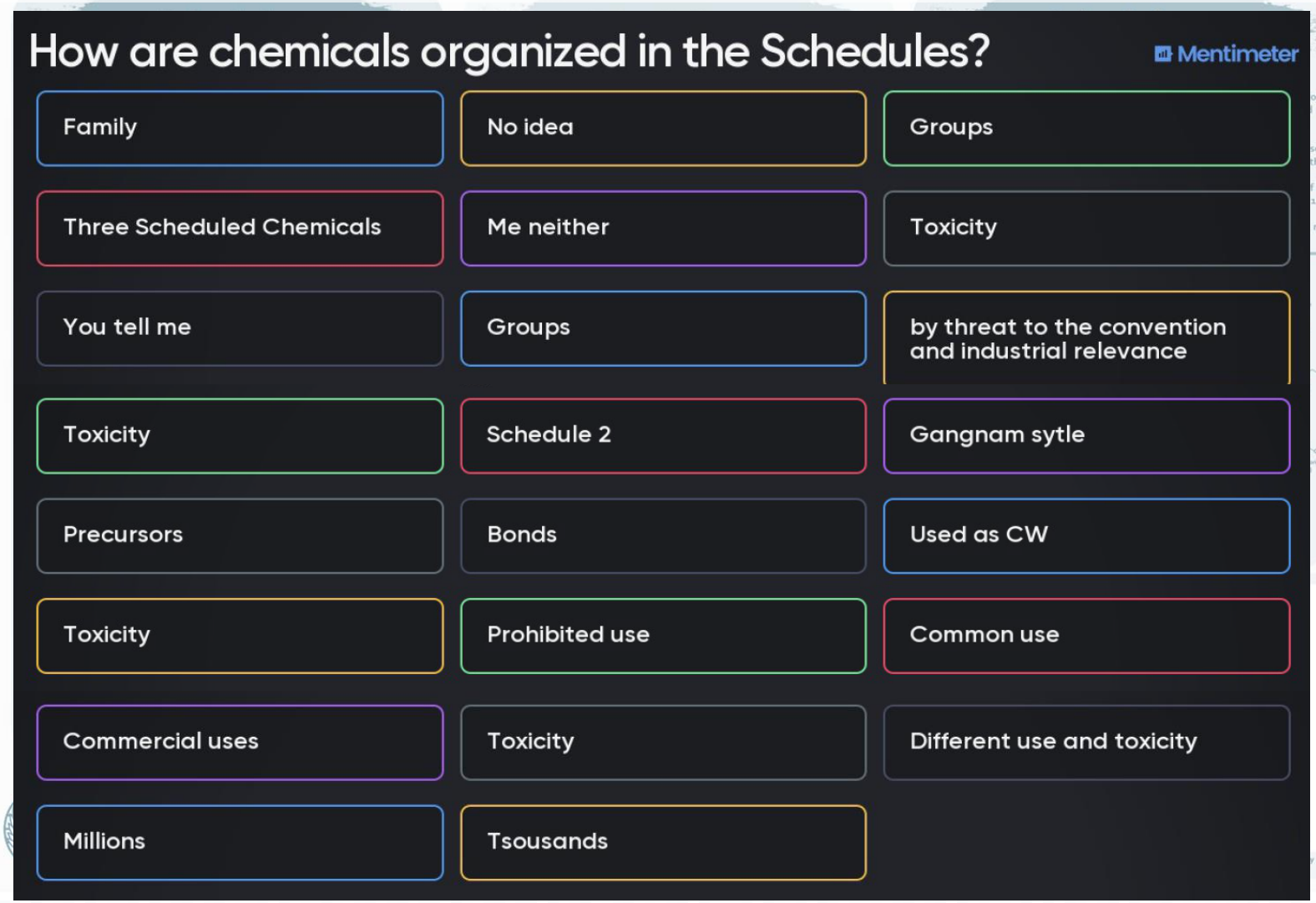






How are chemicals organized in the Schedules?

Answers from Participants



Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Schedule 1

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:

(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:

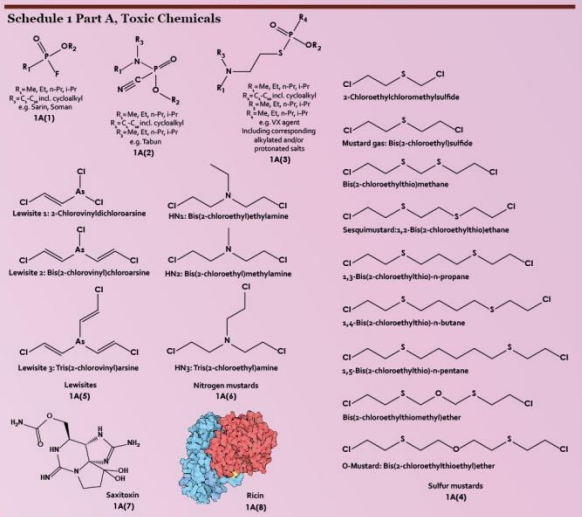
(i) It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparableproperties;

(ii) It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;

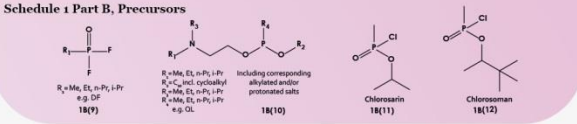
(iii) It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;

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

Schedule 1 Part A, Toxic Chemicals



Schedule 1 Part B, Precursors



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:

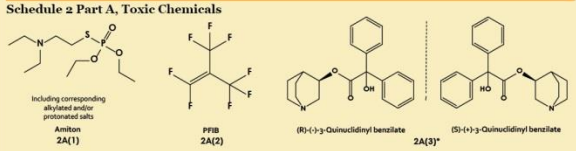
(a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;

(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;

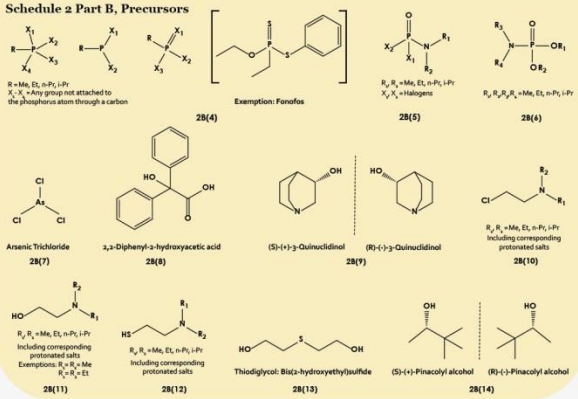
(c) It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;

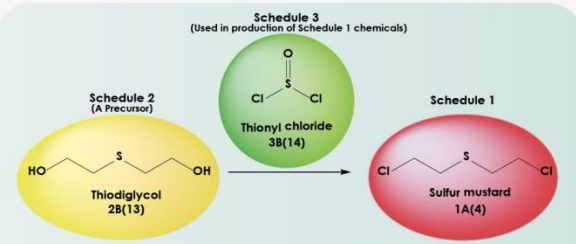
(d) It is not produced in large commercial quantities for purposes not prohibited under this Convention.

Schedule 2 Part A, Toxic Chemicals



Schedule 2 Part B, Precursors





Relationship between Schedules, illustrated with sulfur mustard.

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:

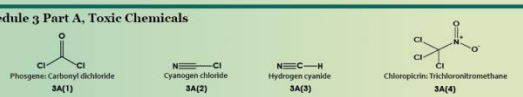
(a) It has been produced, stockpiled or used as a chemical weapon;

(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;

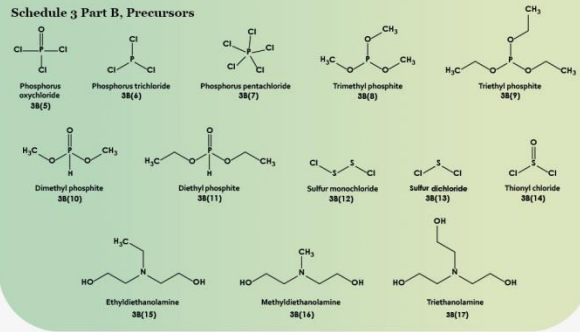
(c) It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, part B;

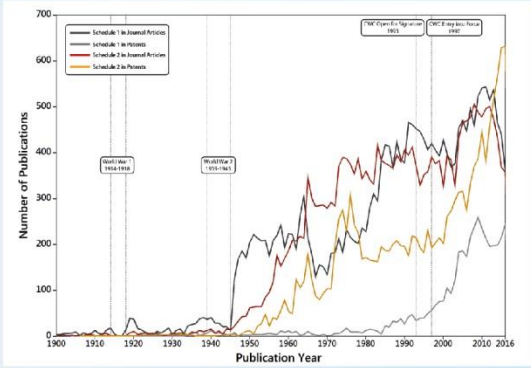
(d) It may be produced in large commercial quantities for purposes not prohibited under this Convention.

Schedule 3 Part A, Toxic Chemicals



Schedule 3 Part B, Precursors





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.

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

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Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Schedule 1

Guidelines for Schedule 1

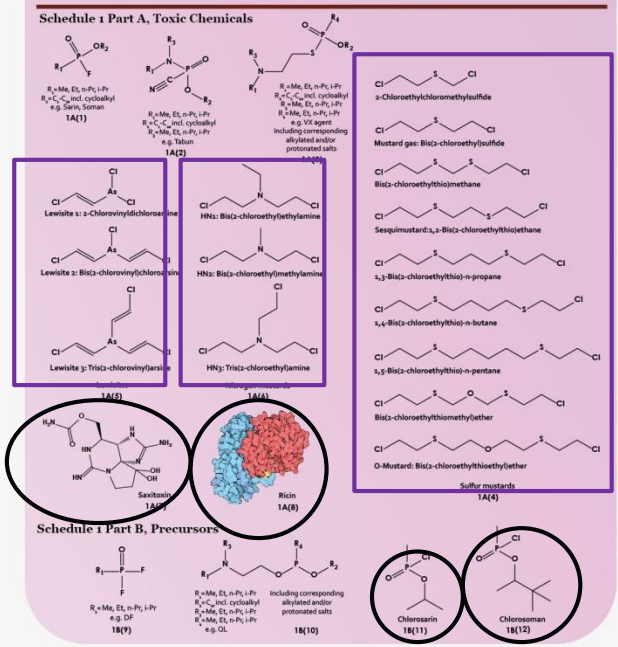
The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

(a) It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;

(b) 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;

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

3 Groups of chemicals
(15 total chemical substances)



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:

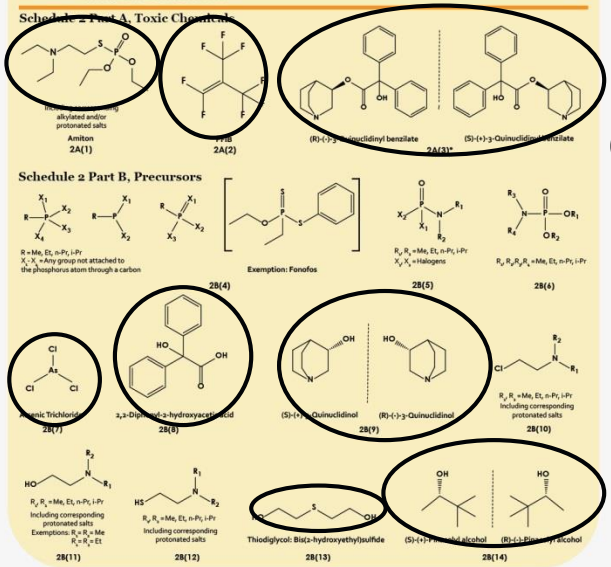
(a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;

(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.

29 Single chemical substances
3 Shown here as pairs of stereoisomers

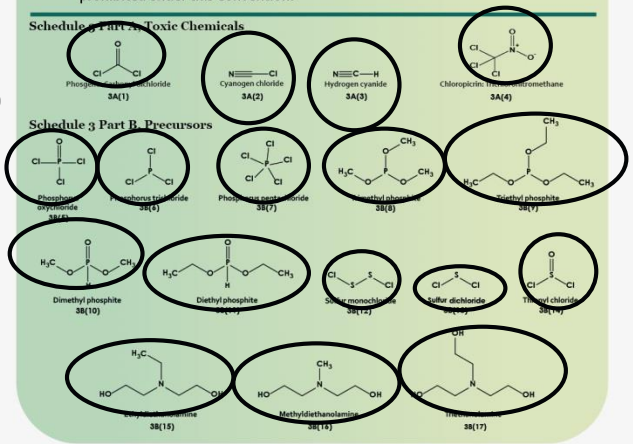


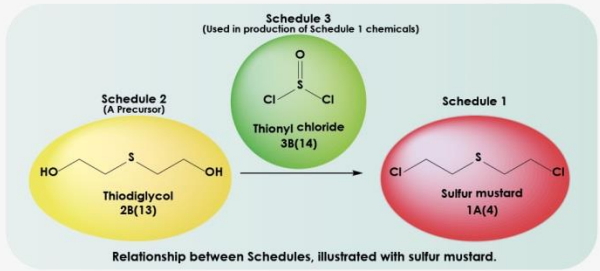
Schedule 3

Guidelines for Schedule 3

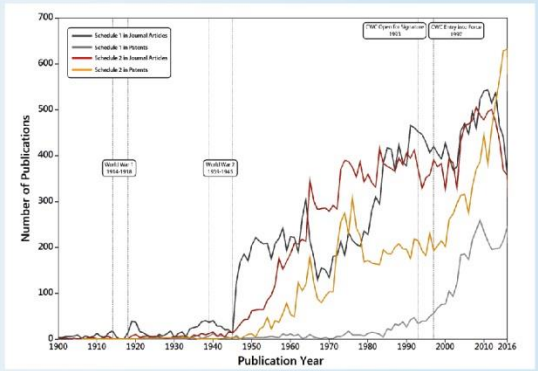
(c) It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, part B;

(d) It may be produced in large commercial quantities for purposes not prohibited under this Convention.





Relationship between Schedules, illustrated with sulfur mustard.



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.

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

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and 11 “families” of chemical weapons agents and precursors

5 in Schedule 1, 6 in Schedule 2

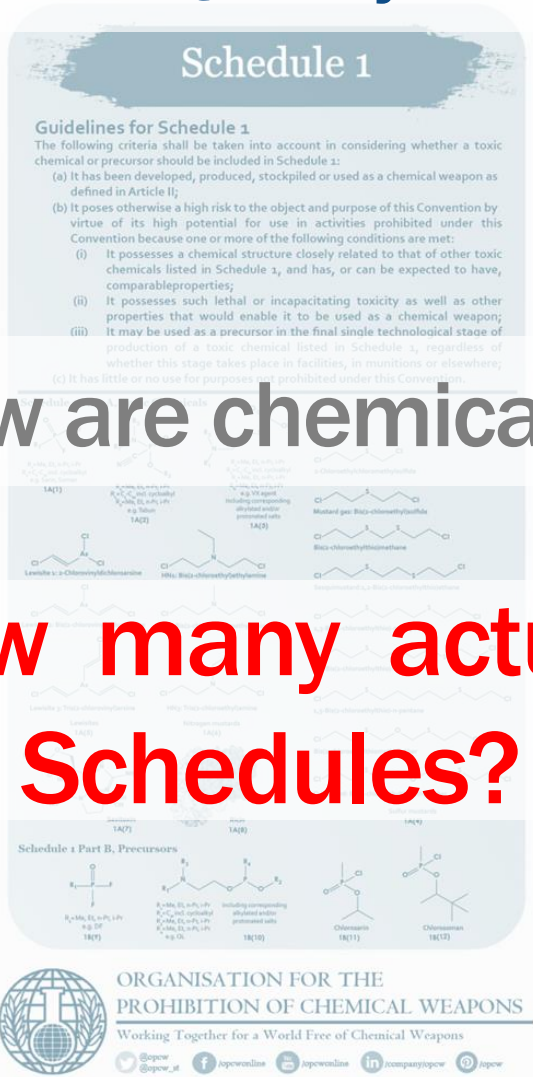
All 11 families cover organophosphorus chemicals (8) or amines (3)

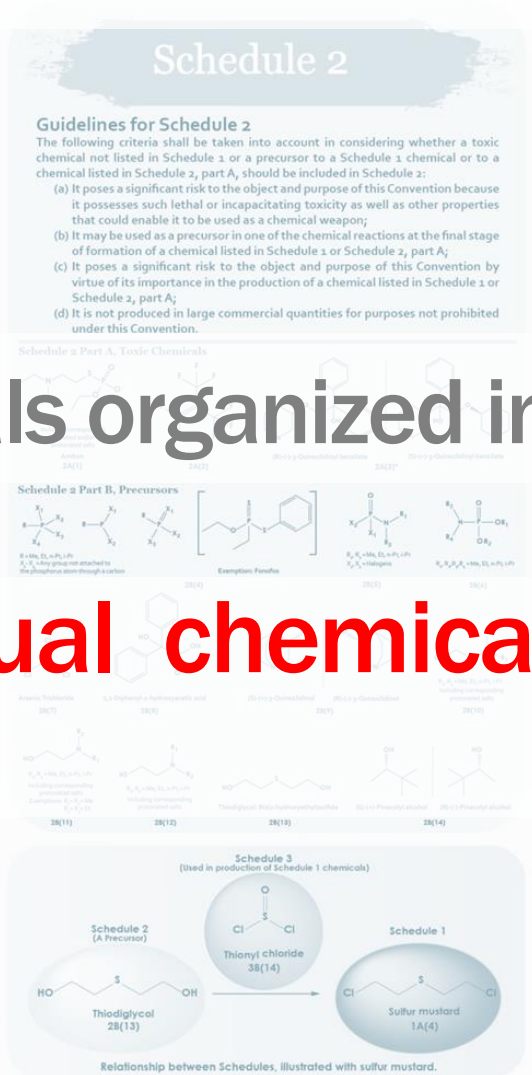
These types of chemicals are also Scheduled as specific chemicals and in groups

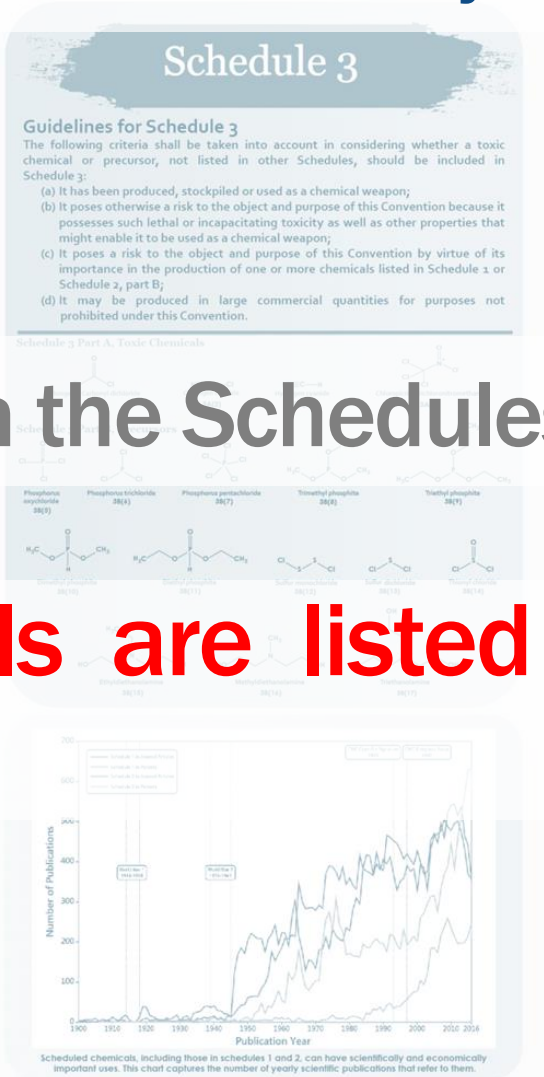
Lets Quickly Review Where we left of from July

How are chemicals organized in the Schedules?

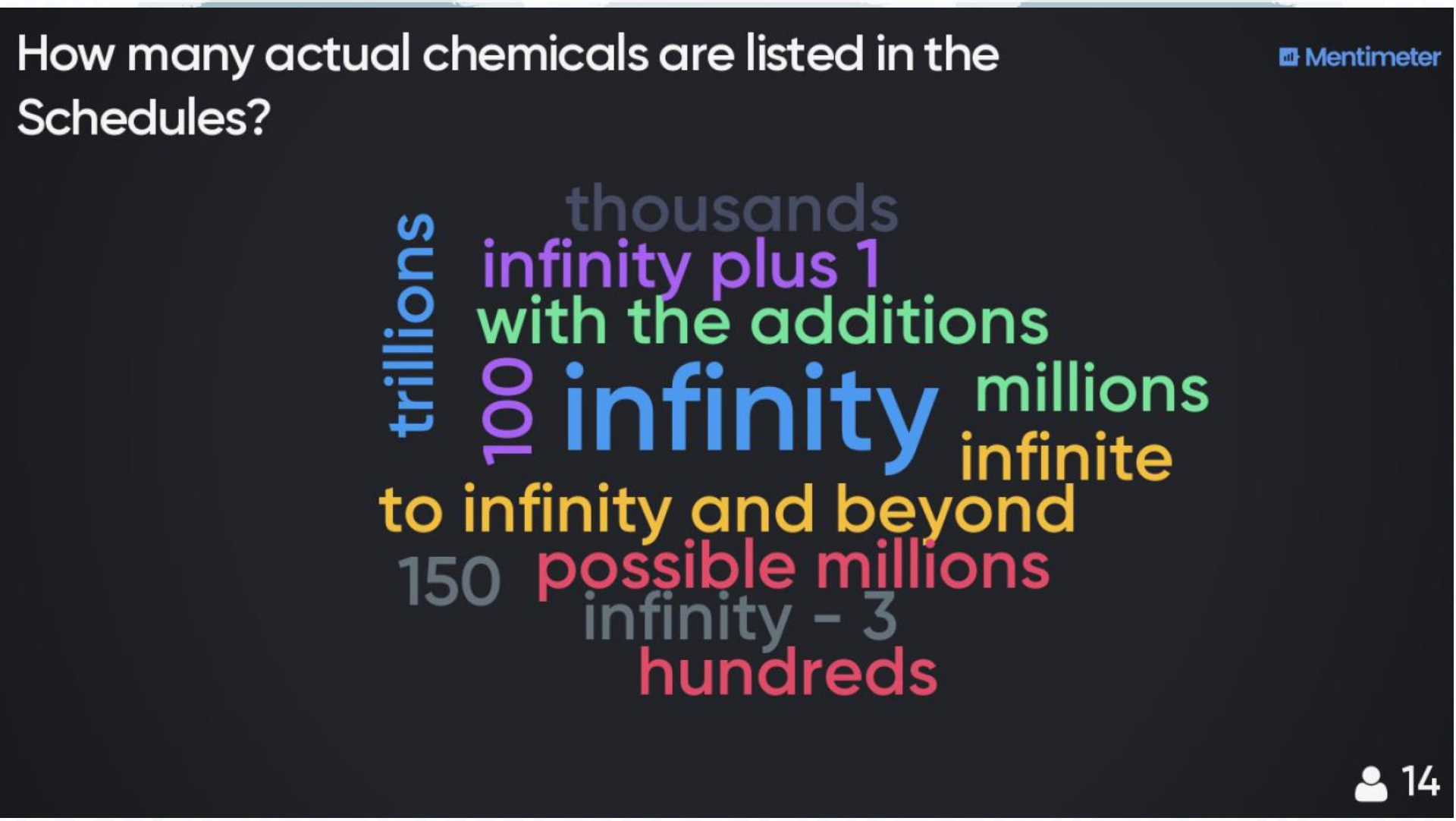
How many actual chemicals are listed in the Schedules?







Answers from Participants



How Many Actual Chemicals are in the Schedules?

B. SCHEDULES OF CHEMICALS

The following Schedules list toxic chemicals and their precursors. For the purpose of implementing this Convention, these Schedules identify chemicals for the application of verification measures according to the provisions of the Verification Annex. Pursuant to Article II, subparagraph 1 (a), these Schedules do not constitute a definition of chemical weapons.

(Whenever reference is made to groups of dialkylated chemicals, followed by a list of alkyl groups in parentheses, all chemicals possible by all possible combinations of alkyl groups listed in the parentheses are considered as listed in the respective Schedule as long as they are not explicitly exempted. A chemical marked "*" on Schedule 2, part A, is subject to special thresholds for declaration and verification, as specified in Part VII of the Verification Annex.)

Schedule 1 (CAS registry number)

A. Toxic chemicals:

(1) O-Alkyl (≤C_{10}, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates

e.g. Sarin: O-Isopropyl methylphosphonofluoridate (107-44-8)
Soman: O-Pinacolyl methylphosphonofluoridate (96-64-0)

(2) O-Alkyl (≤C_{10}, incl. cycloalkyl) N,N-dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidocyanidates

e.g. Tabun: O-Ethyl N,N-dimethyl phosphoramidocyanidate (77-81-6)

(3) O-Alkyl (H or ≤C_{10}, incl. cycloalkyl) S-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonothiolates and corresponding alkylated or protonated salts

e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (50782-69-9)

(4) Sulfur mustards:

2-Chloroethylchloromethylsulfide (2625-76-5)
Mustard gas: Bis(2-chloroethyl)sulfide (505-60-2)
Bis(2-chloroethylthio)methane (63869-13-6)
Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane (3563-36-8)
1,3-Bis(2-chloroethylthio)-n-propane (63905-10-2)
1,4-Bis(2-chloroethylthio)-n-butane (142868-93-7)
1,5-Bis(2-chloroethylthio)-n-pentane (142868-94-8)
Bis(2-chloroethylthiomethyl)ether (63918-90-1)
O-Mustard: Bis(2-chloroethylthioethyl)ether (63918-89-8)

(5) Lewisites:

Lewisite 1: 2-Chlorovinyldichloroarsine (541-25-3)
Lewisite 2: Bis(2-chlorovinyl)chloroarsine (40334-69-8)
Lewisite 3: Tris(2-chlorovinyl)arsine (40334-70-1)

(6) Nitrogen mustards:

HN1: Bis(2-chloroethyl)ethylamine (538-07-8)
HN2: Bis(2-chloroethyl)methylamine (51-75-2)
HN3: Tris(2-chloroethyl)amine (555-77-1)

(7) Saxitoxin (35523-89-8)

(8) Ricin (9009-86-3)

B. Precursors:

(9) Alkyl (Me, Et, n-Pr or i-Pr) phosphonyldifluorides

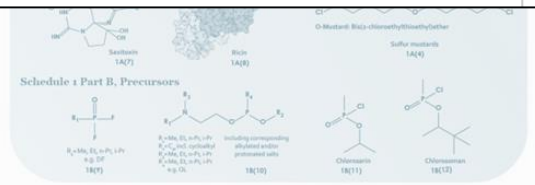
e.g. DF: Methylphosphonyldifluoride (676-99-3)

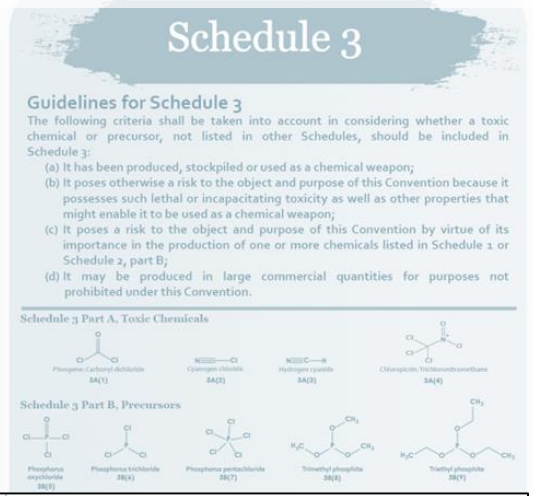
(10) O-Alkyl (H or ≤C_{10}, incl. cycloalkyl) O-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonites and corresponding alkylated or protonated salts

e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite (57856-11-8)

(11) Chlorosarin: O-Isopropyl methylphosphonochloridate (1445-76-7)

(12) Chlorosoman: O-Pinacolyl methylphosphonochloridate (7040-57-5)





Schedule 2

A. Toxic chemicals:

(1) Amiton: O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate and corresponding alkylated or protonated salts (78-53-5)

(2) PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene (382-21-8)

(3) BZ: 3-Quinuclidinyl benzilate (*) (6581-06-2)

B. Precursors:

(4) Chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms,

e.g. Methylphosphonyl dichloride (676-97-1)
Dimethyl methylphosphonate (756-79-6)

Exemption: Fonofos: O-Ethyl S-phenyl ethylphosphonothiolothionate (944-22-9)

(5) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides

(6) Dialkyl (Me, Et, n-Pr or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates

(7) Arsenic trichloride (7784-34-1)

(8) 2,2-Diphenyl-2-hydroxyacetic acid (76-93-7)

(9) Quinuclidin-3-ol (1619-34-7)

(10) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts

(11) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-ols and corresponding protonated salts

Exemptions: N,N-Dimethylaminoethanol and corresponding protonated salts (108-01-0)
N,N-Diethylaminoethanol and corresponding protonated salts (100-37-8)

(12) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-thiols and corresponding protonated salts

(13) Thiodiglycol: Bis(2-hydroxyethyl)sulfide (111-48-8)

(14) Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol (464-07-3)

Schedule 3

A. Toxic chemicals:

(1) Phosgene: Carbonyl dichloride (75-44-5)

(2) Cyanogen chloride (506-77-4)

(3) Hydrogen cyanide (74-90-8)

(4) Chloropicrin: Trichloronitromethane (76-06-2)

B. Precursors:

(5) Phosphorus oxychloride (10025-87-3)

(6) Phosphorus trichloride (7719-12-2)

(7) Phosphorus pentachloride (10026-13-8)

(8) Trimethyl phosphite (121-45-9)

(9) Triethyl phosphite (122-52-1)

(10) Dimethyl phosphite (868-85-9)

(11) Diethyl phosphite (762-04-9)

(12) Sulfur monochloride (10025-67-9)

(13) Sulfur dichloride (10545-99-0)

(14) Thionyl chloride (7719-09-7)

(15) Ethyldiethanolamine (139-87-7)

(16) Methyldiethanolamine (105-59-9)

(17) Triethanolamine (102-71-6)

OPCW

How Many Actual Chemicals are in the Schedules?

B. SCHEDULES OF CHEMICALS

The following Schedules list toxic chemicals and their precursors. For the purpose of implementing this Convention, these Schedules identify chemicals for the application of verification measures according to the provisions of the Verification Annex. Pursuant to Article II, subparagraph 1 (a), these Schedules do not constitute a definition of chemical weapons.

(Whenever reference is made to groups of dialkylated chemicals, followed by a list of alkyl groups in parentheses, all chemicals possible by all possible combinations of alkyl groups listed in the parentheses are considered as listed in the respective Schedule as long as they are not explicitly exempted. A chemical marked "*" on Schedule 2, part A, is subject to special thresholds for declaration and verification, as specified in Part VII of the Verification Annex.)

Schedule 1 (CAS registry number)

A. Toxic chemicals:

(1) O-Alkyl (≤C_{10}, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates

e.g. Sarin: O-Isopropyl methylphosphonofluoridate (107-44-8)
Soman: O-Pinacolyl methylphosphonofluoridate (96-64-0)

(2) O-Alkyl (≤C_{10}, incl. cycloalkyl) N,N-dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidocyanidates

e.g. Tabun: O-Ethyl N,N-dimethyl phosphoramidocyanidate (77-81-6)

(3) O-Alkyl (H or ≤C_{10}, incl. cycloalkyl) S-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonothiolates and corresponding alkylated or protonated salts

e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (50782-69-9)

(4) Sulfur mustards:

2-Chloroethylchloromethylsulfide (2625-76-5)
Mustard gas: Bis(2-chloroethyl)sulfide (505-60-2)
Bis(2-chloroethylthio)methane (63869-13-6)
Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane (3563-36-8)
1,3-Bis(2-chloroethylthio)-n-propane (63905-10-2)
1,4-Bis(2-chloroethylthio)-n-butane (142868-93-7)
1,5-Bis(2-chloroethylthio)-n-pentane (142868-94-8)
Bis(2-chloroethylthiomethyl)ether (63918-90-1)
O-Mustard: Bis(2-chloroethylthioethyl)ether (63918-89-8)

descriptions/formulas

(5) Lewisites:

Lewisite 1: 2-Chlorovinyldichloroarsine (541-25-3)
Lewisite 2: Bis(2-chlorovinyl)chloroarsine (40334-69-8)
Lewisite 3: Tris(2-chlorovinyl)arsine (40334-70-1)

(6) Nitrogen mustards:

HN1: Bis(2-chloroethyl)ethylamine (538-07-8)
HN2: Bis(2-chloroethyl)methylamine (51-75-2)
HN3: Tris(2-chloroethyl)amine (555-77-1)

(7) Saxitoxin (35523-89-8)

(8) Ricin (9009-86-3)

B. Precursors:

(9) [illegible], Et, n-Pr or i-Pr) phosphonyldifluorides

e.g. DF: Methylphosphonyldifluoride (676-99-3)

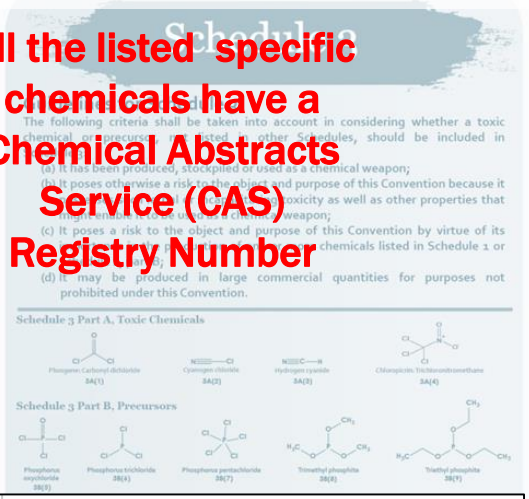
(10) O-Alkyl (H or ≤C_{10}, incl. cycloalkyl) O-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonites and corresponding alkylated or protonated salts

e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite (57856-11-8)

(11) Chlorosarin: O-Isopropyl methylphosphonochloridate (1445-76-7)

(12) Chlorosoman: O-Pinacolyl methylphosphonochloridate (7040-57-5)

All the listed specific chemicals have a Chemical Abstracts Service (CAS) Registry Number



Schedule 2

A. Toxic chemicals:

(1) Amiton: O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate and corresponding alkylated or protonated salts (78-53-5)

(2) PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene (382-21-8)

(3) BZ: 3-Quinuclidinyl benzilate (*) (6581-06-2)

B. Precursors:

(4) Chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms,

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Dimethyl methylphosphonate (756-79-6)

Exemption: Fonofos: O-Ethyl S-phenyl ethylphosphonothiolothionate (944-22-9)

(5) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides

(6) Dialkyl (Me, Et, n-Pr or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates

(7) Arsenic trichloride (7784-34-1)

(8) 2,2-Diphenyl-2-hydroxyacetic acid (76-93-7)

(9) Quinuclidin-3-ol (1619-34-7)

(10) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts

(11) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-ols and corresponding protonated salts

Exemptions: N,N-Dimethylaminoethanol and corresponding protonated salts (108-01-0)
N,N-Diethylaminoethanol and corresponding protonated salts (100-37-8)

(12) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-thiols and corresponding protonated salts

(13) Thiodiglycol: Bis(2-hydroxyethyl)sulfide (111-48-8)

(14) Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol (464-07-3)

Specific chemicals

Schedule 3

A. Toxic chemicals:

(1) Phosgene: Carbonyl dichloride (75-44-5)

(2) Cyanogen chloride (506-77-4)

(3) Hydrogen cyanide (74-90-8)

(4) Chloropicrin: Trichloronitromethane (76-06-2)

B. Precursors:

(5) Phosphorus oxychloride (10025-87-3)

(6) Phosphorus trichloride (7719-12-2)

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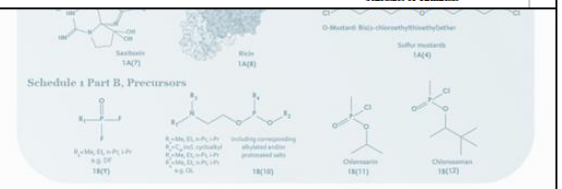

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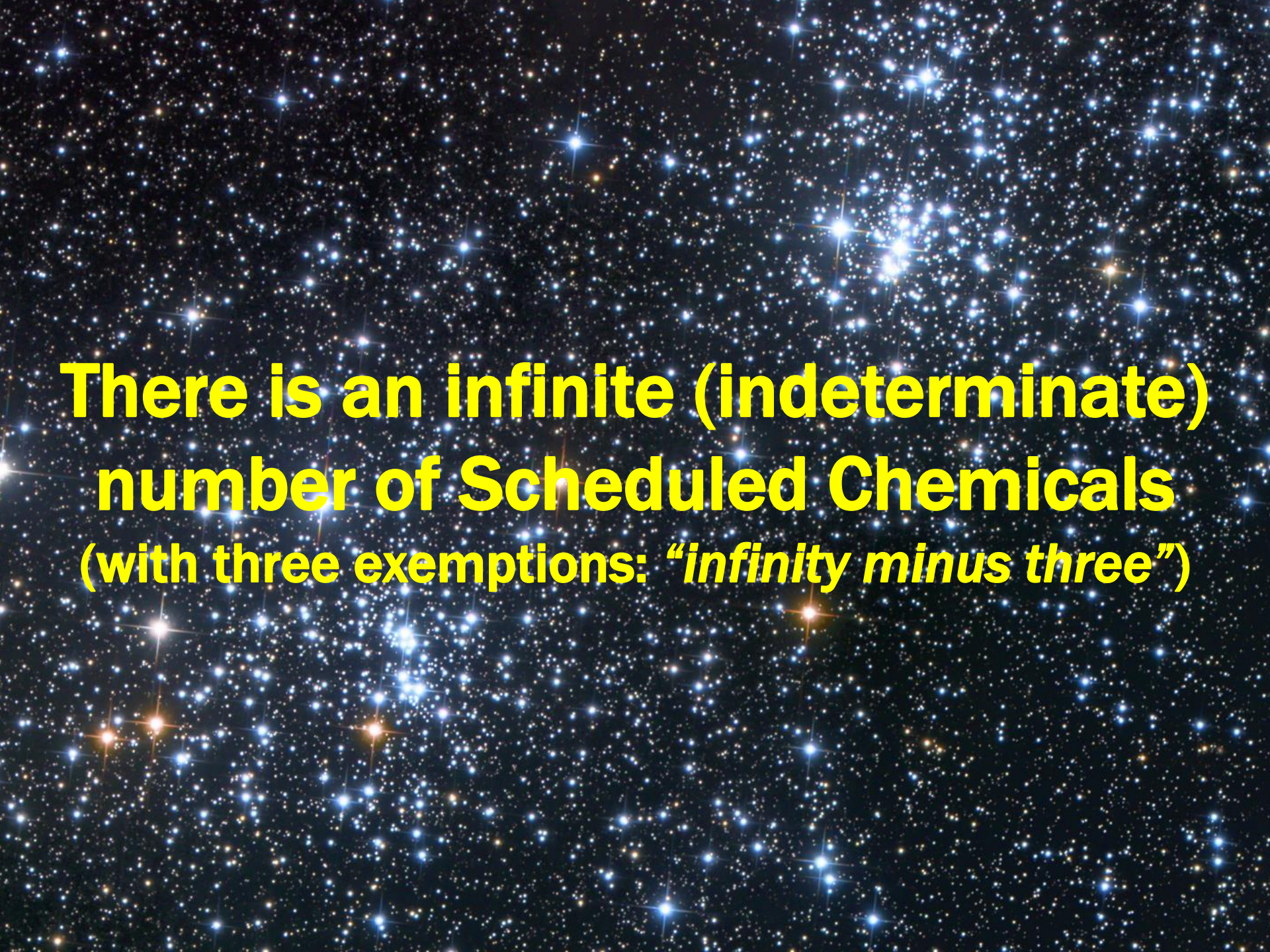
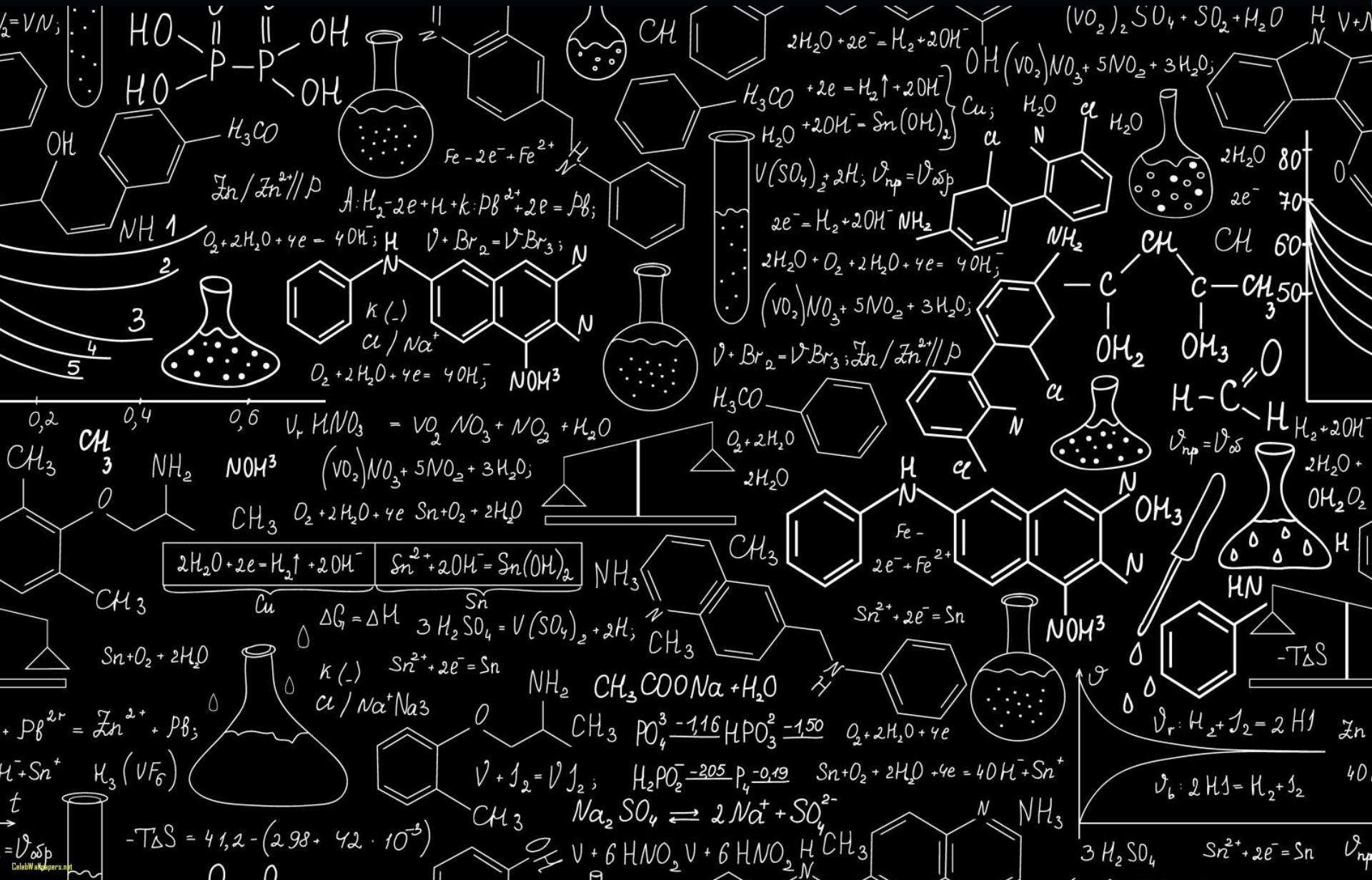

There is an infinite (indeterminate) number of Scheduled Chemicals
(with three exemptions: "infinity minus three")

To Make Sense of all of this Requires a Discussion of Chemistry (Atoms, Molecules and Math!)



What do Scheduled Chemicals Look Like?

Schedule 1

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:

(a) It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;

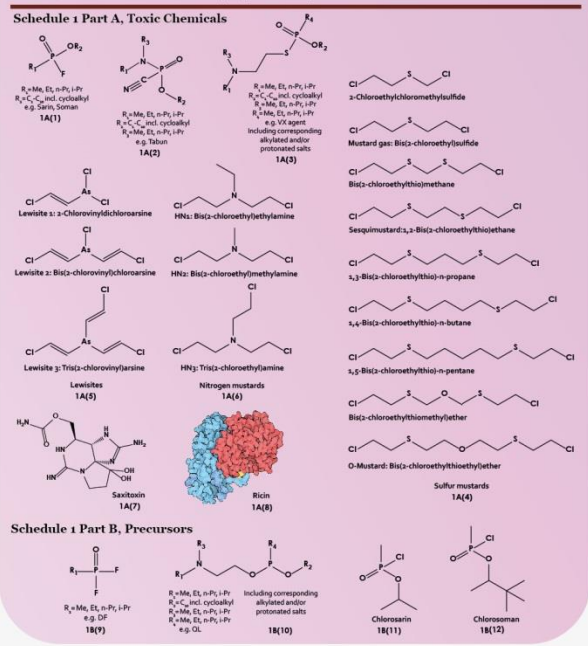
(b) It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:

(i) It possesses a chemical structure closely related to that of other toxic 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

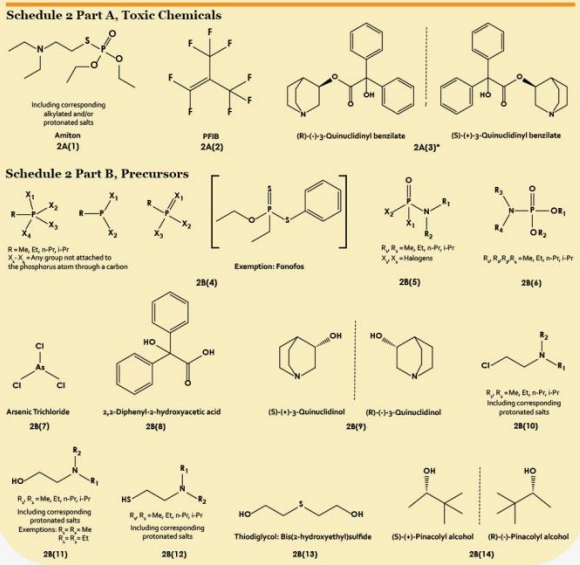
The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:

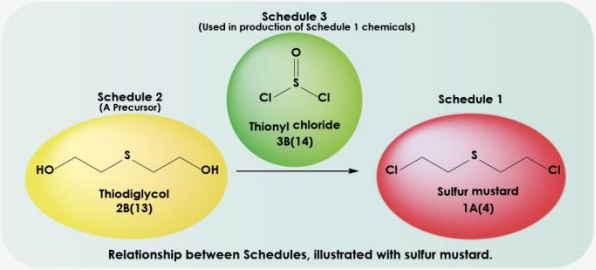
(a) It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;

(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 3

Guidelines for Schedule 3

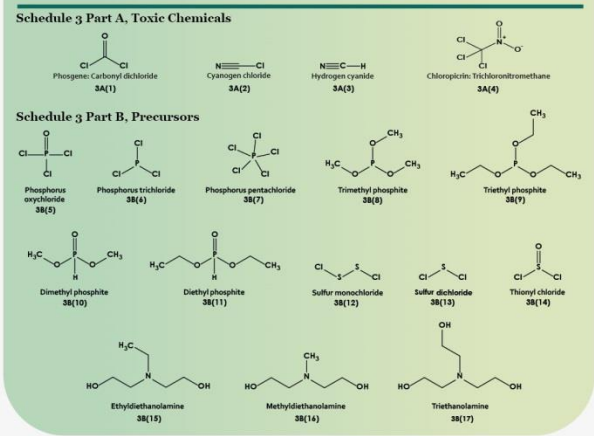
The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

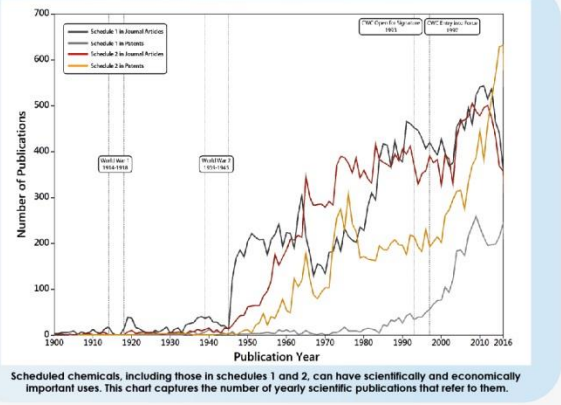
(a) It has been produced, stockpiled or used as a chemical weapon;

(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.





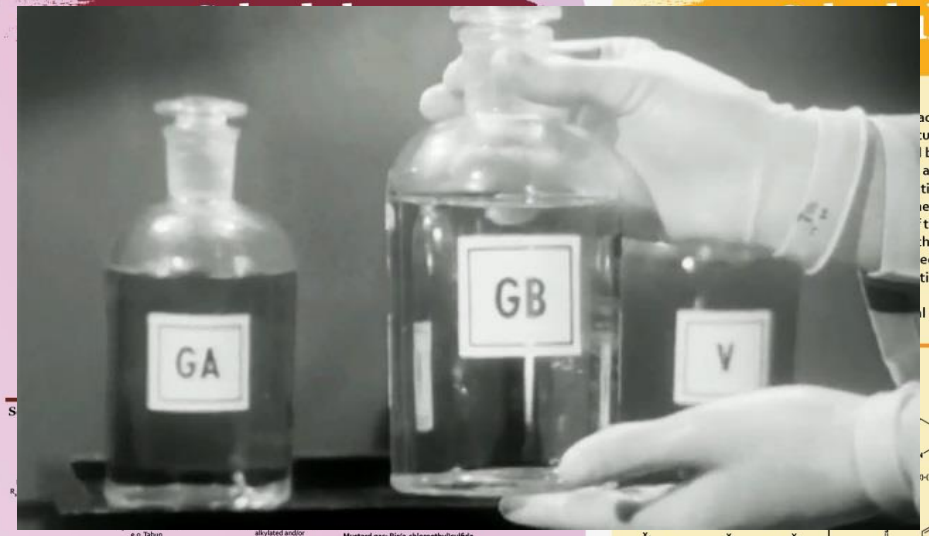
Scheduled chemicals, including those in schedules 1 and 2, can have scientifically and economically important uses. This chart captures the number of yearly scientific publications that refer to them.

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

@opcw @opcw_st /opcwonline /opcwonline /company/opcw /opcw

What do Scheduled Chemicals Look Like?



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.

Schedule 3 Part A, Toxic Chemicals

Phosgene: Carbonyl dichloride 3A(1) · Cyanogen chloride 3A(2) · Hydrogen cyanide 3A(3) · Chloropicrin: Trichloronitromethane 3A(4)

Schedule 3 Part B, Precursors

Schedule 1 Part B, Precursors

Lewisite 1: 2-Chlorovinyldichloroarsine · Lewisite 2: Bis(2-chlorovinyl)chloroarsine · Lewisite 3: Tris(2-chlorovinyl)arsine · Lewisites 1A(5) · HN1: Bis(2-chloroethyl)ethylamine · HN2: Bis(2-chloroethyl)methylamine · HN3: Tris(2-chloroethyl)amine · 1A(6) · Saxitoxin 1A(7) · Ricin 1A(8) · Mustard gas: Bis(2-chloroethyl)sulfide · Bis(2-chloroethylthio)methane · 1A(2) · 1A(3) · 1B(9) · 1B(10)

ORGANISATION FO
PROHIBITION OF C
Working Together for a World Free of Chemical Weapons

@opcw @opcw_st · /opcwonline · /opcwonline · /company/opcw · /opcw

Relationship between Schedules, illustrated with sulfur mustard.

important uses. This chart captures the number of yearly scientific publications that refer to them.

What do Scheduled Chemicals Look Like?

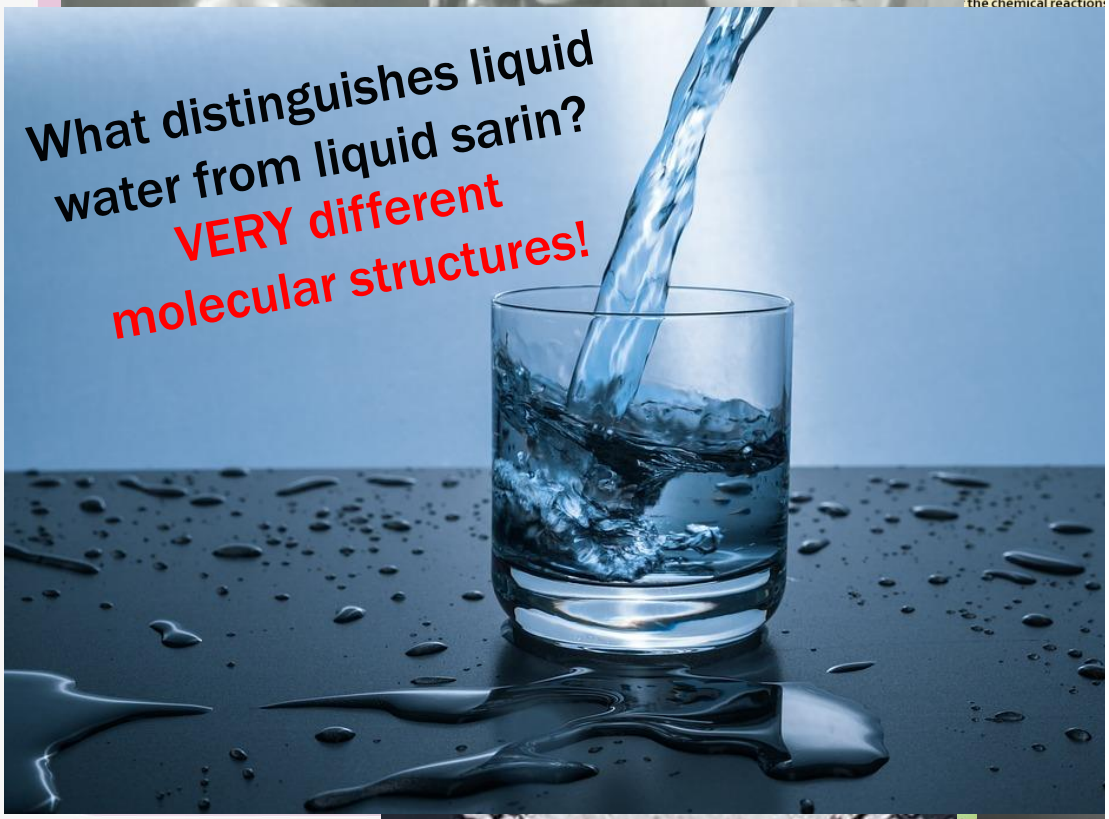
Schedule 3

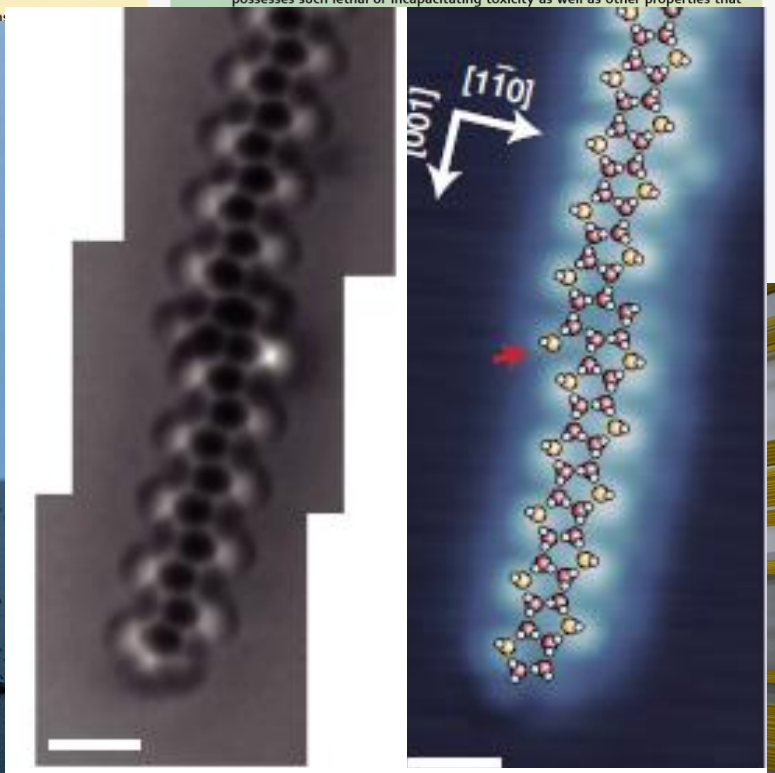
Guidelines for Schedule 3

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:

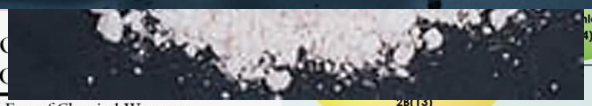
(a) It has been produced, stockpiled or used as a chemical weapon;

(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





Water molecules!
DOI: 10.1038/ncomms14313



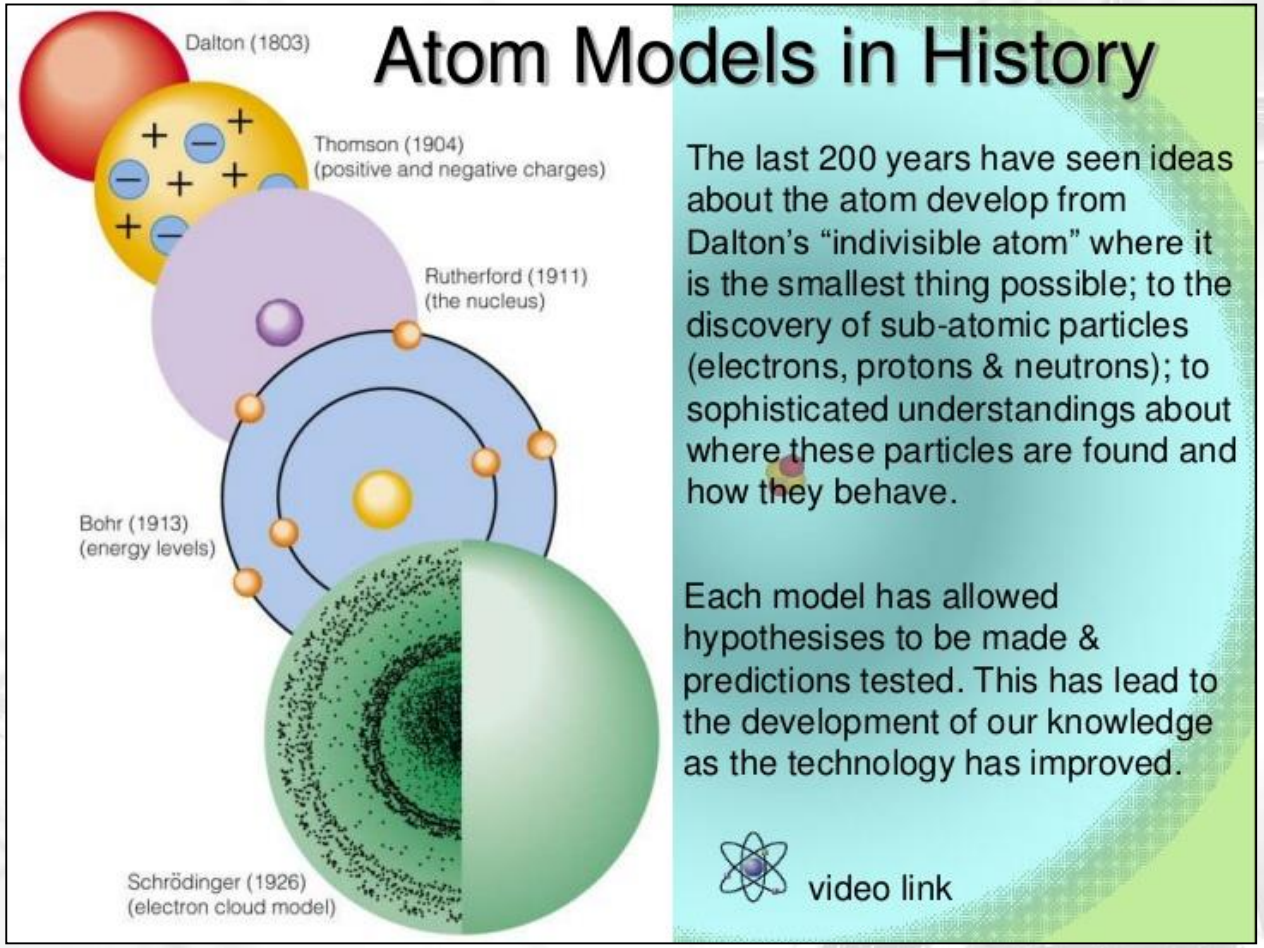
ORGANISATION FO
PROHIBITION OF C
Working Together for a World Free of Chemical Weapons

@opcw @opcw_st /opcwonline /opcwonline /company/opcw /opcw

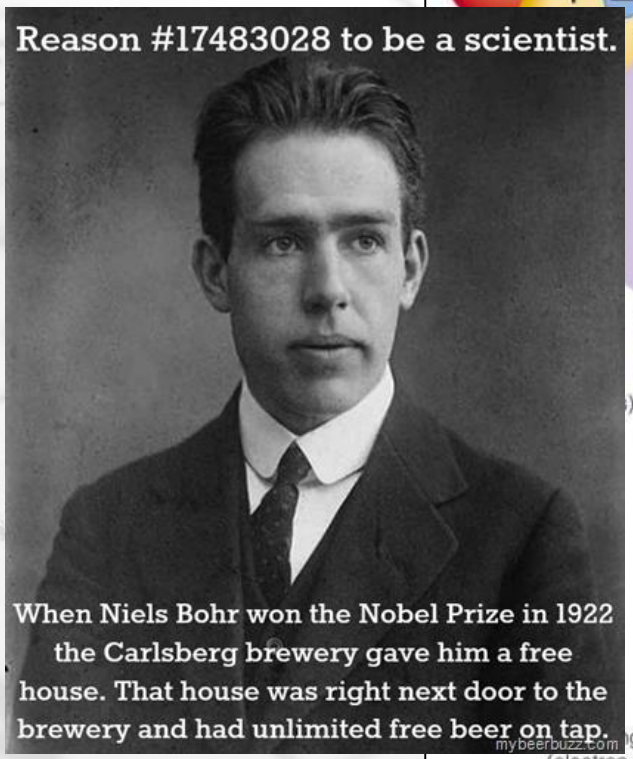
Relationship between Schedules, illustrated with sulfur mustard.

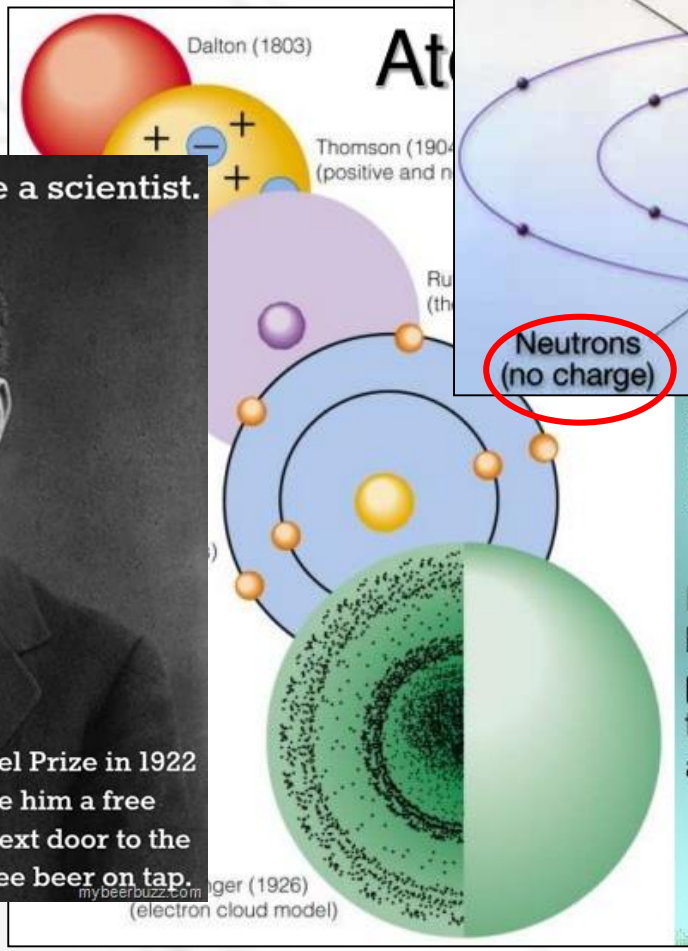
important uses. This chart captures the number of yearly scientific publications that refer to them.

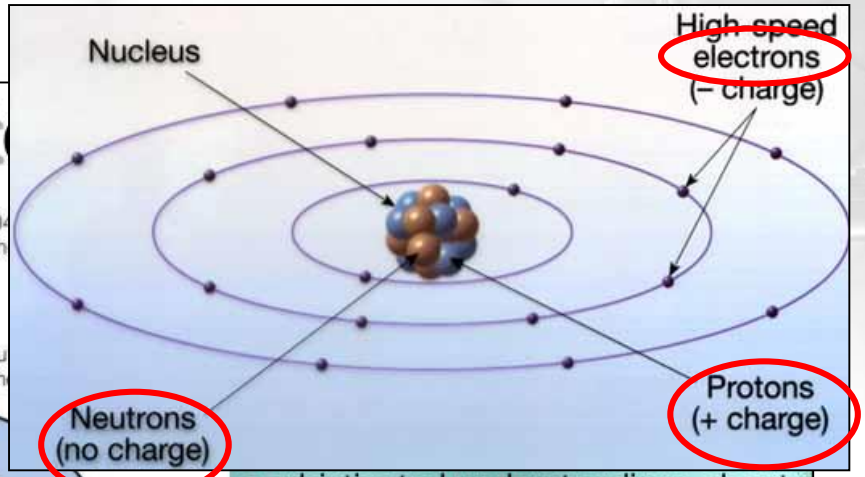
Recognizing How a Chemical "Behaves" is all About the Atoms!



Recognizing How a Chemical "Behaves" is all About the Atoms!





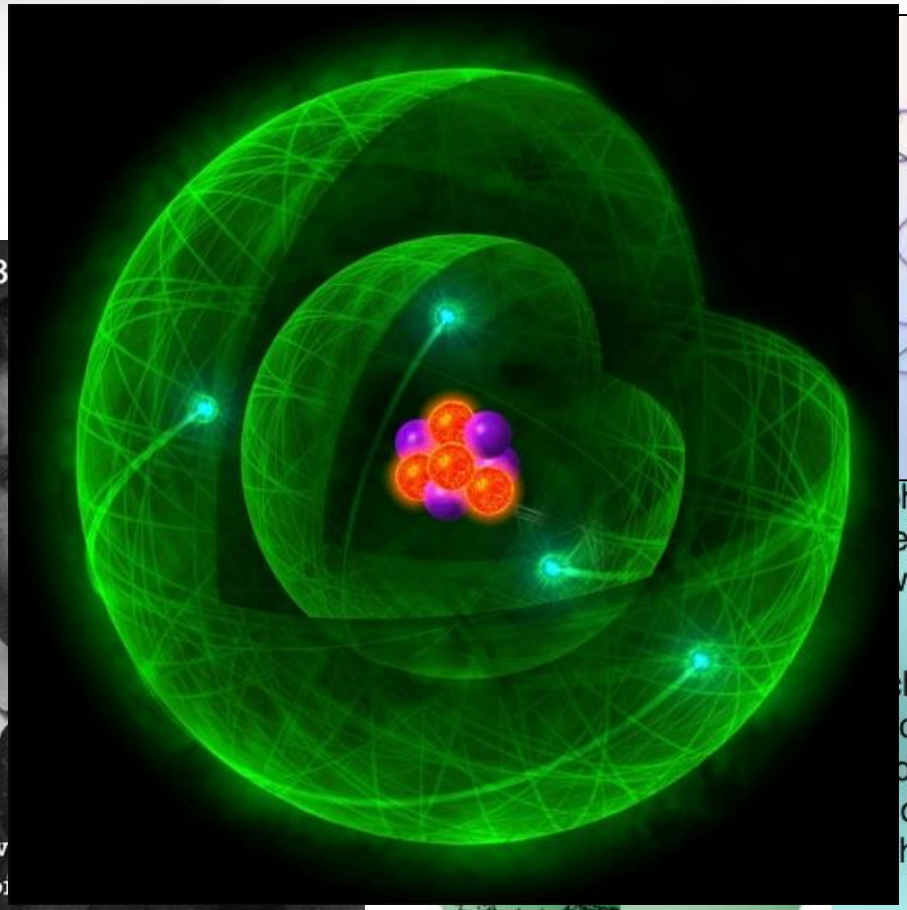


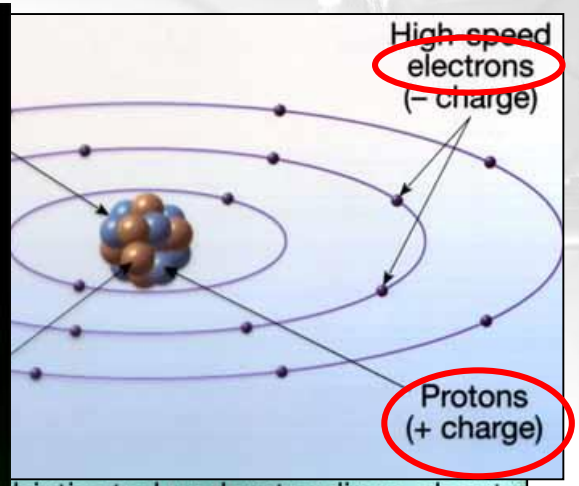
sophisticated understandings about where these particles are found and how they behave.

Each model has allowed hypothesises to be made & predictions tested. This has lead to the development of our knowledge as the technology has improved.

video link

Recognizing How a Chemical "Behaves" is all About the Atoms!





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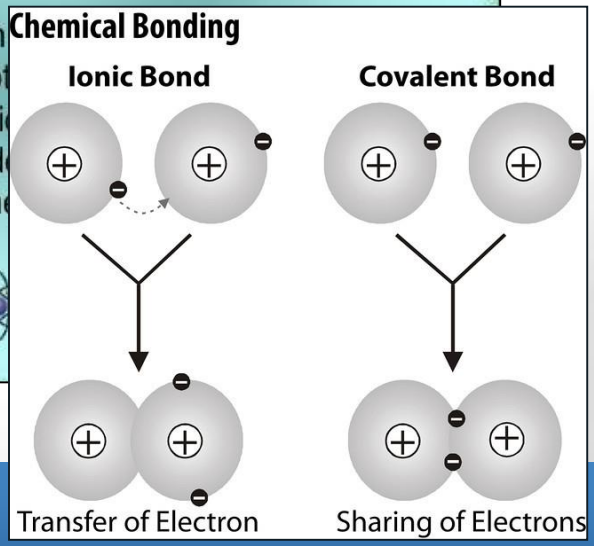
ere these particles are found and
they behave.

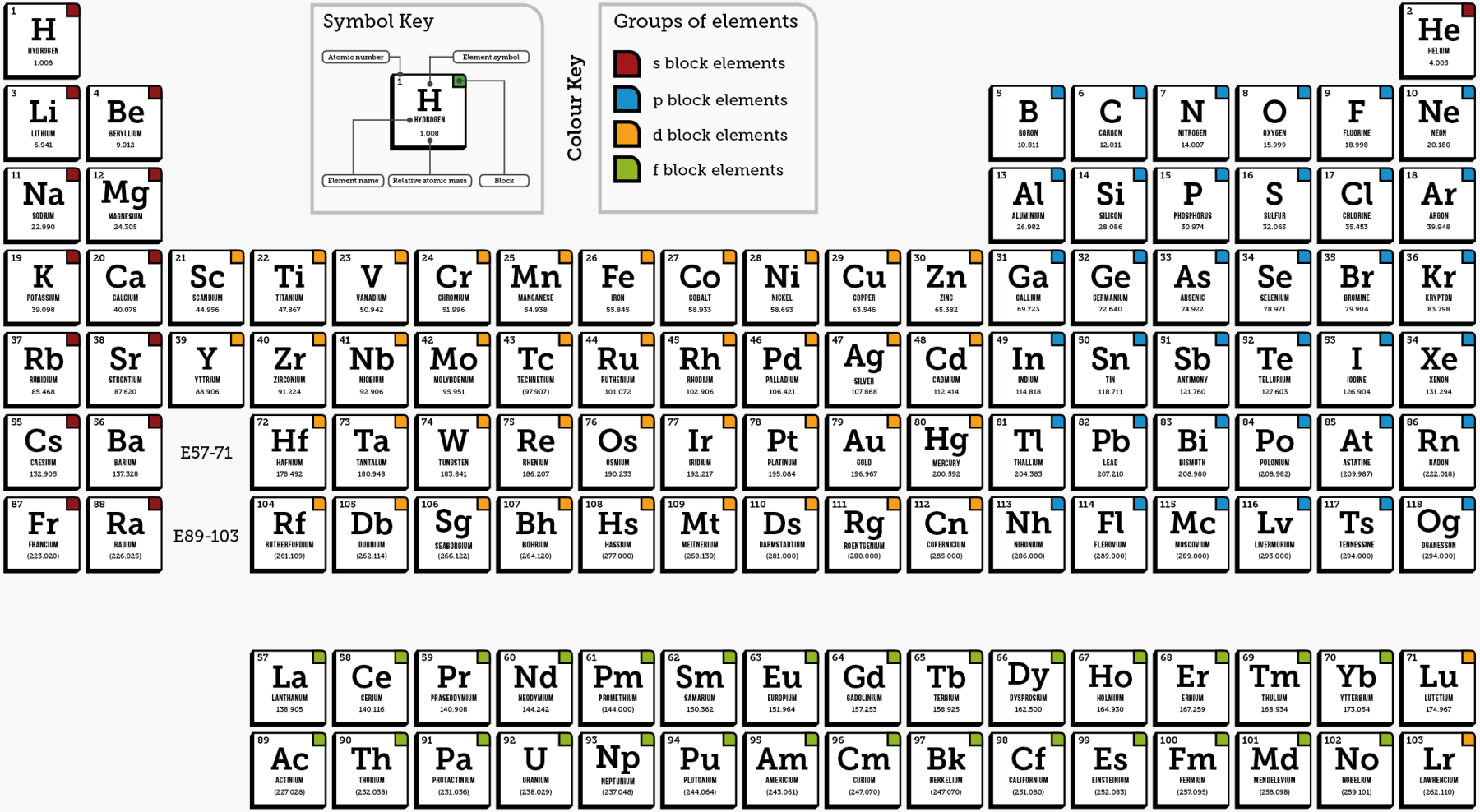


ger (1926)
(electron cloud model)

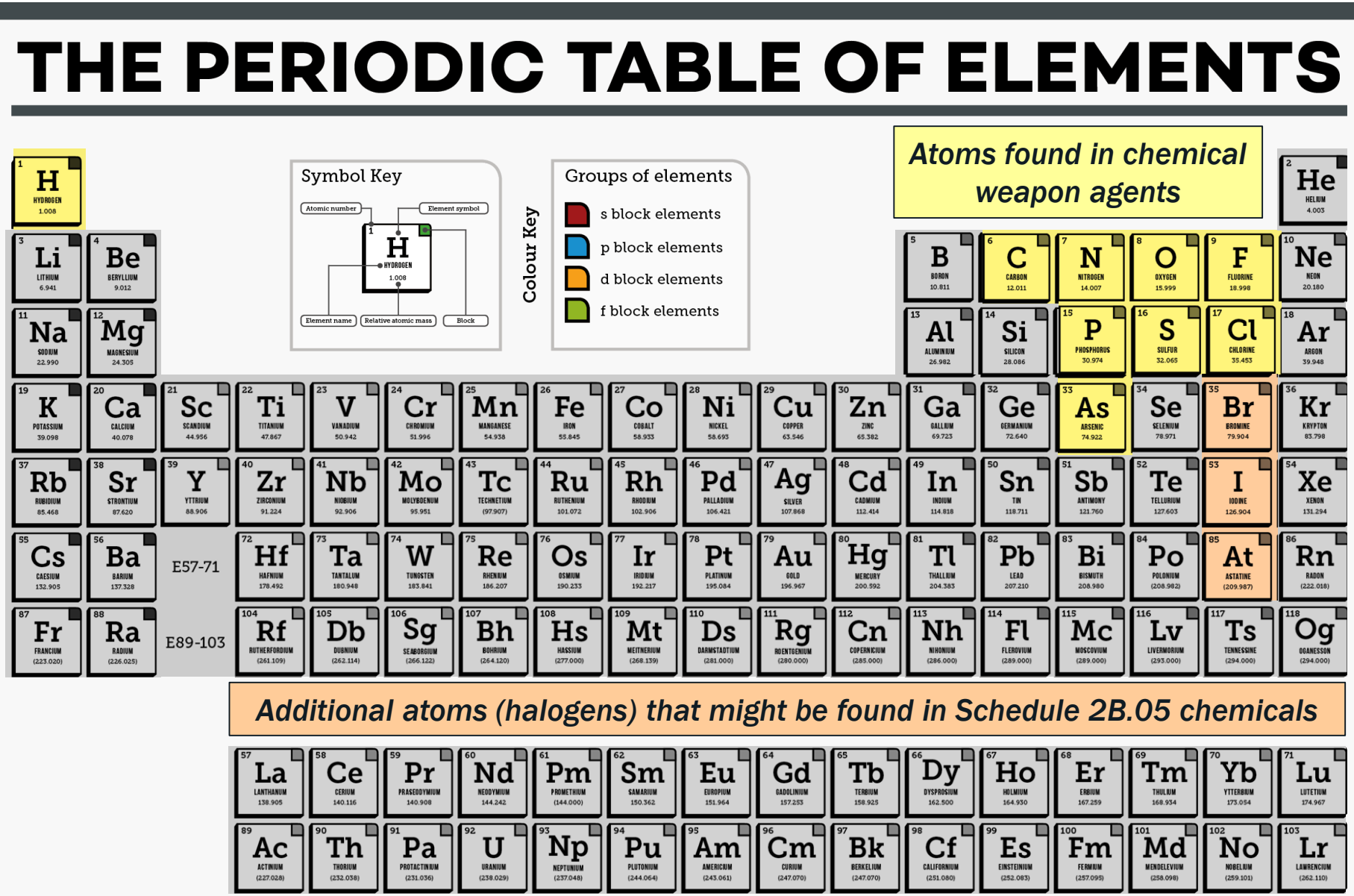
OPCW

There are 118 Types of Atoms (at least for now...)

THE PERIODIC TABLE OF ELEMENTS

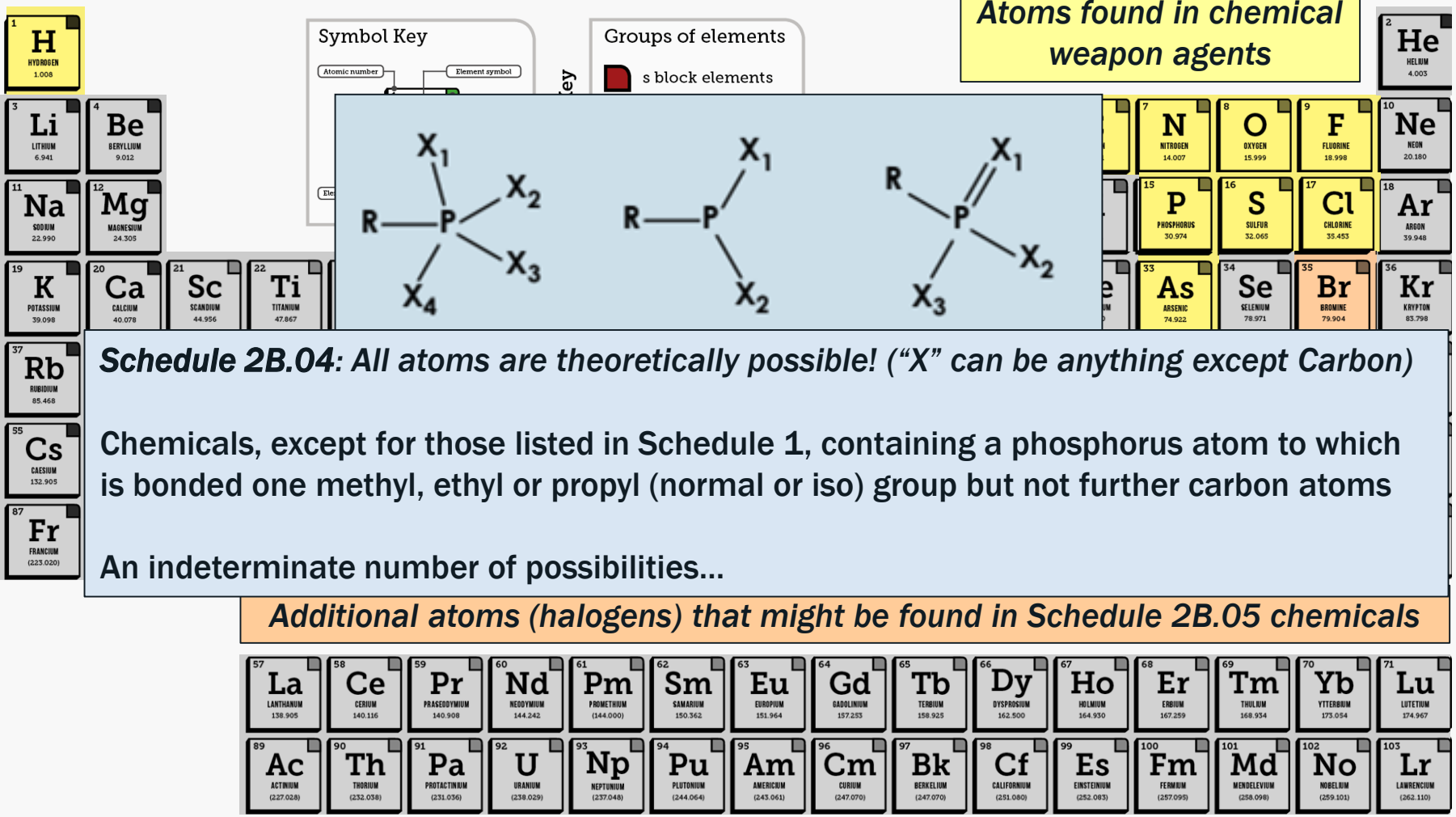


There are 118 Types of Atoms (at least for now...)



There are 118 Types of Atoms (at least for now...)

THE PERIODIC TABLE OF ELEMENTS

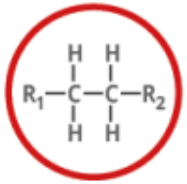


Chemicals are Defined by the Types of Atoms and Bonds

FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.

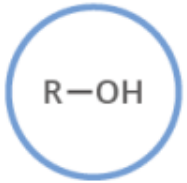
HYDROCARBONS | SIMPLE OXYGEN HETEROATOMICS | HALOGEN HETEROATOMICS | CARBONYL COMPOUNDS | NITROGEN-BASED | SULFUR-BASED | AROMATIC



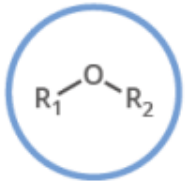
ALKANE
Naming: -ane
e.g. ethane

ALKENE
Naming: -ene
e.g. ethene

ALKYNE
Naming: -yne
e.g. ethyne



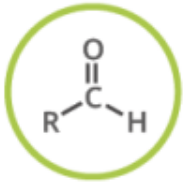
ALCOHOL
Naming: -ol
e.g. ethanol



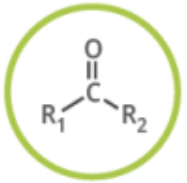
ETHER
Naming: -oxy -ane
e.g. methoxyethane

EPOXIDE
Naming: -ene oxide
e.g. ethene oxide

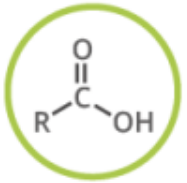
HALOALKANE
Naming: halo-
e.g. chloroethane



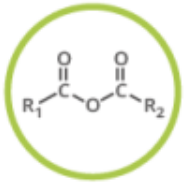
ALDEHYDE
Naming: -al
e.g. ethanal



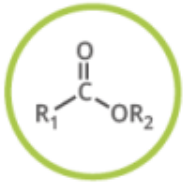
KETONE
Naming: -one
e.g. propanone



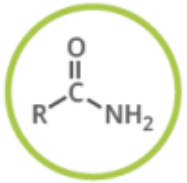
CARBOXYLIC ACID
Naming: -oic acid
e.g. ethanoic acid



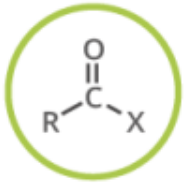
ACID ANHYDRIDE
Naming: -oic anhydride
e.g. ethanoic anhydride



ESTER
Naming: -yl -oate
e.g. ethyl ethanoate



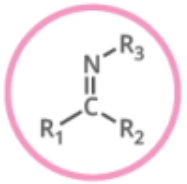
AMIDE
Naming: -amide
e.g. ethanamide



ACYL HALIDE
Naming: -oyl halide
e.g. ethanoyl chloride

AMINE
Naming: -amine
e.g. ethanamine

NITRILE
Naming: -nitrile
e.g. ethanenitrile

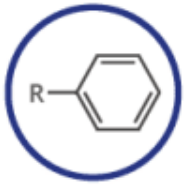


IMINE
Naming: -imine
e.g. ethanimine

ISOCYANATE
Naming: -yl isocyanate
e.g. ethyl isocyanate

AZO COMPOUND
Naming: azo-
e.g. azoethane

THIOL
Naming: -thiol
e.g. methanethiol



ARENE
Naming: -yl benzene
e.g. ethyl benzene

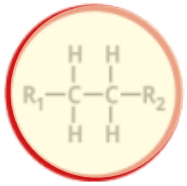
Chemicals are Defined by the Types of Atoms and Bonds

Specific examples listed in the Schedules
(Possible to have the others in scheduled chemicals as well)

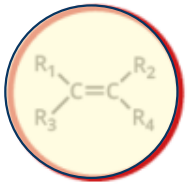
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES.
FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.

HYDROCARBONS | SIMPLE OXYGEN HETEROATOMICS | HALOGEN HETEROATOMICS | CARBONYL COMPOUNDS | NITROGEN-BASED | SULFUR-BASED | AROMATIC

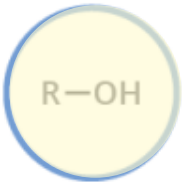


ALKANE
Naming: -ane
e.g. ethane

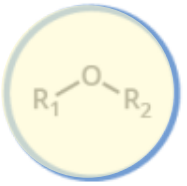


ALKENE
Naming: -ene
e.g. ethene

ALKYNE
Naming: -yne
e.g. ethyne



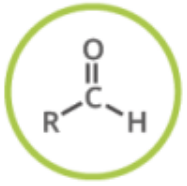
ALCOHOL
Naming: -ol
e.g. ethanol



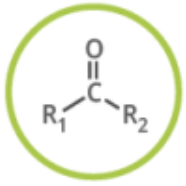
ETHER
Naming: -oxy -ane
e.g. methoxyethane

EPOXIDE
Naming: -ene oxide
e.g. ethene oxide

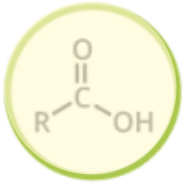
HALOALKANE
Naming: halo-
e.g. chloroethane



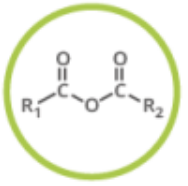
ALDEHYDE
Naming: -al
e.g. ethanal



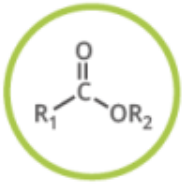
KETONE
Naming: -one
e.g. propanone



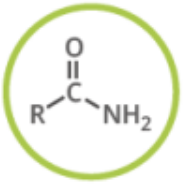
CARBOXYLIC ACID
Naming: -oic acid
e.g. ethanoic acid



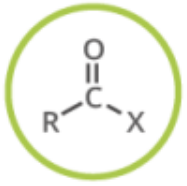
ACID ANHYDRIDE
Naming: -oic anhydride
e.g. ethanoic anhydride



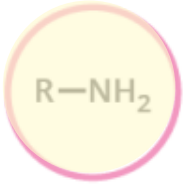
ESTER
Naming: -yl -oate
e.g. ethyl ethanoate



AMIDE
Naming: -amide
e.g. ethanamide

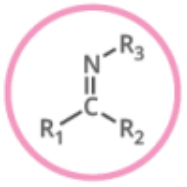


ACYL HALIDE
Naming: -oyl halide
e.g. ethanoyl chloride



AMINE
Naming: -amine
e.g. ethanamine

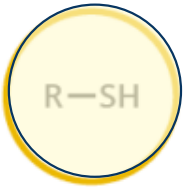
NITRILE
Naming: -nitrile
e.g. ethanenitrile



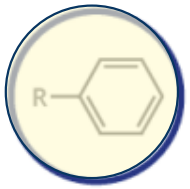
IMINE
Naming: -imine
e.g. ethanimine

ISOCYANATE
Naming: -yl isocyanate
e.g. ethyl isocyanate

AZO COMPOUND
Naming: azo-
e.g. azoethane

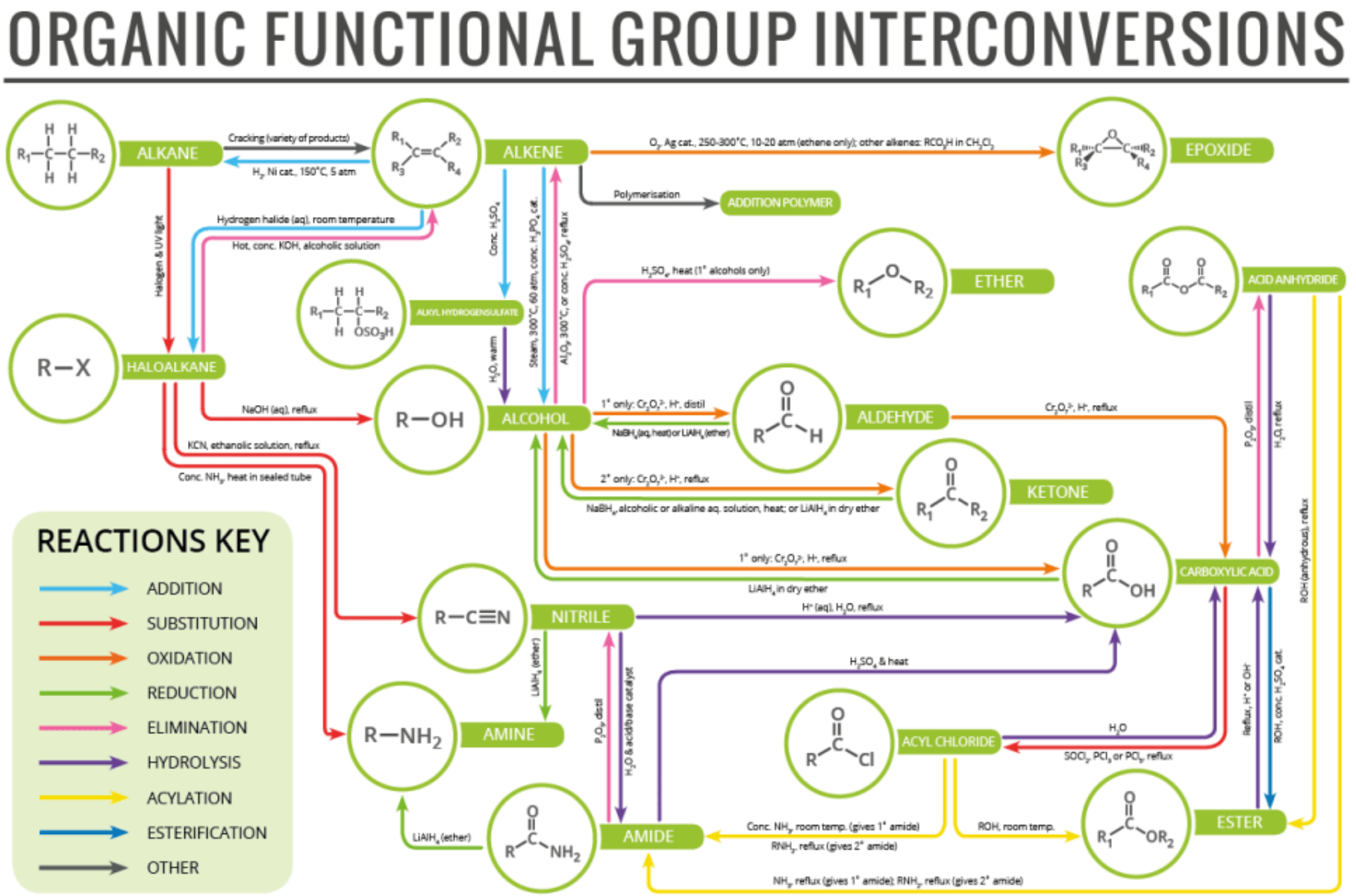


THIOL
Naming: -thiol
e.g. methanethiol

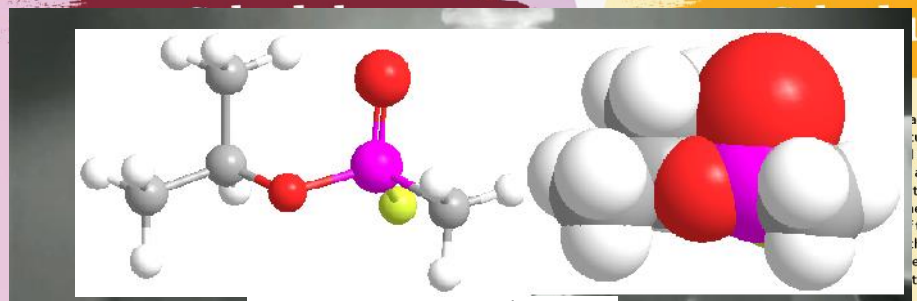


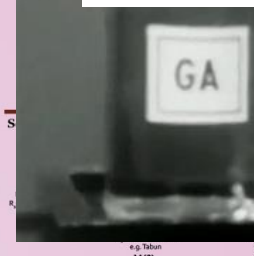
ARENE
Naming: -yl benzene
e.g. ethyl benzene

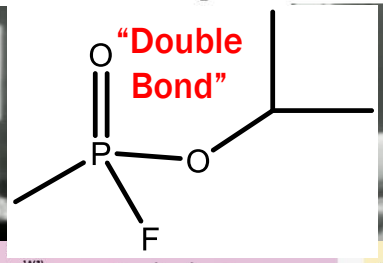
Chemical Behavior is Dictated by the Types of Atoms and Bonds

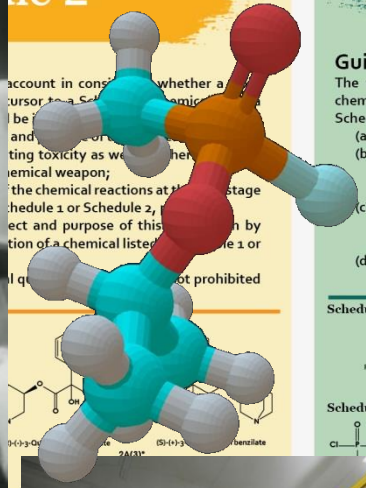


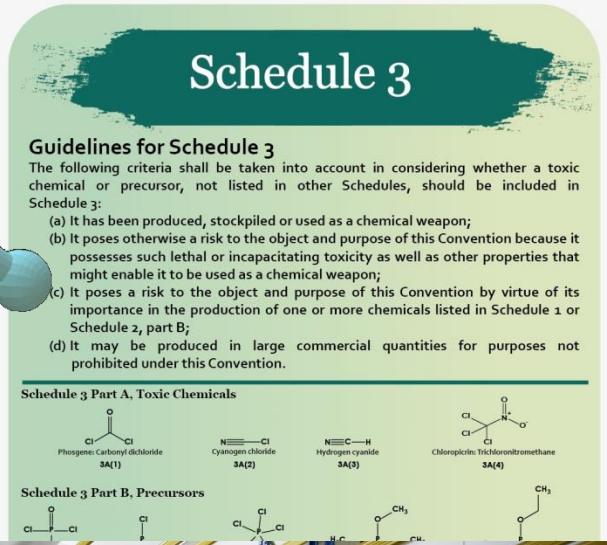
What do Scheduled Chemicals Look Like?

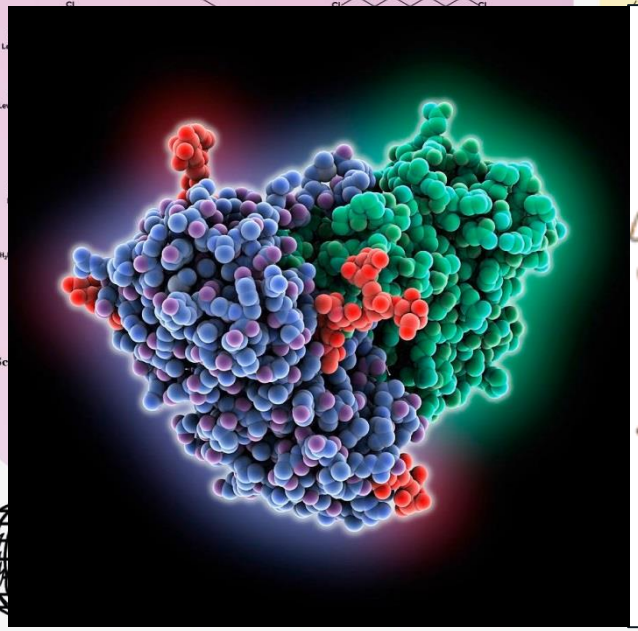


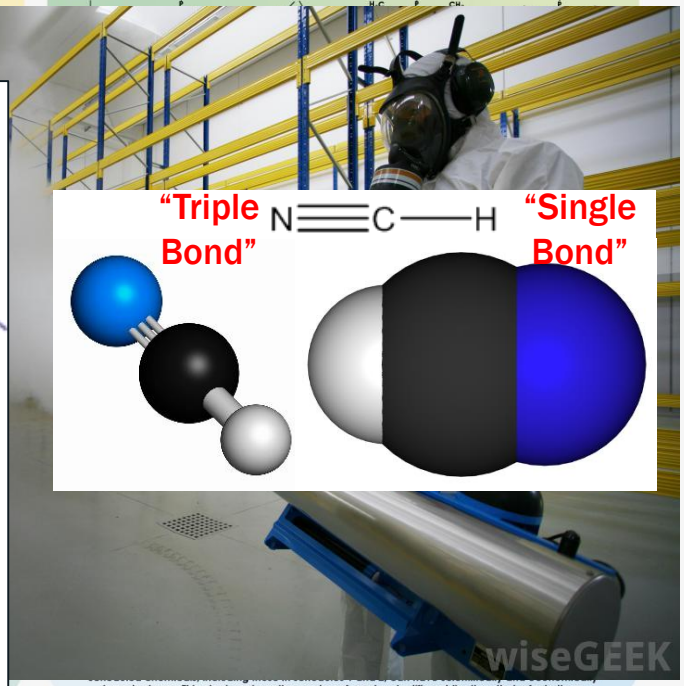












Visualising and Reading Molecular Structures

Created by Maria Hemme and Sofia Sola Sancho (Office of Strategy and Policy)

OPCW

Colour scheme of your model kit

Colour Code for Chemical Elements typically used in models

Carbon (C)	Hydrogen (H)	Sulfur (S)
Nitrogen (N)	Phosphorus (P)	Arsenic (As)
Chorine (Cl)	Fluorine (F)	Oxygen (O)

Single bond

Double bond

In the Structures of Relevance to the Annex on Chemicals:

- Carbon atoms (C) have four bonds
  - If less than four bonds are shown in shorthand, the missing bonds are always C to H
- Chlorine and Fluorine atoms (Cl and F) have one bond
- Hydrogen atoms (H) have one bond
- Nitrogen atoms (N) have three or four bonds
  - four bonds are only for the "salt" form
- Oxygen atoms (O) have two bonds
- Phosphorus and Arsenic atoms (P and As) can have three, four, five or six bonds
  - In the form of a nerve agent P has five bonds - three single bonds and one double bond
- Sulfur (S) can have two, four or six bonds

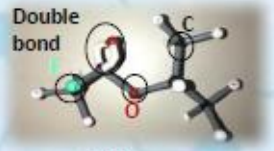
"salt form"

Models → Translation → "Shorthand" structures

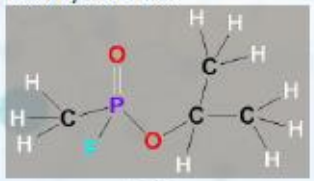
Representation of chemical structures using plastic models. Each "ball" represents an atom of a chemical elements identified by colour. The atoms are linked by single (in grey) or double (in white) bonds.

Graphical representation. These pictures translate the colour of the atoms into the chemical element associated to it, and illustrate the connection between the atoms. This is an intermediate representation to the "shorthand " used by chemists.

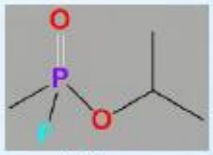
This is a format often used by chemists. It allows bonds between carbon atoms (C) to be shown as connected lines: C atoms that are located at each point where a line connects to other lines or where a line terminates. Additionally, bonds between C and H are not shown for easier visualisation of the structure. Only C-H bonds are hidden, all other bonds are shown.



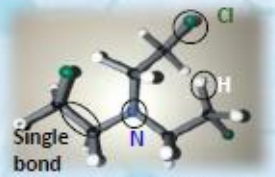
Sarin



Sarin

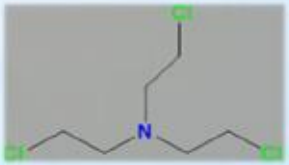


Sarin



Nitrogen mustard (HN-3)

Nitrogen mustard (HN-3)



Nitrogen mustard (HN-3)

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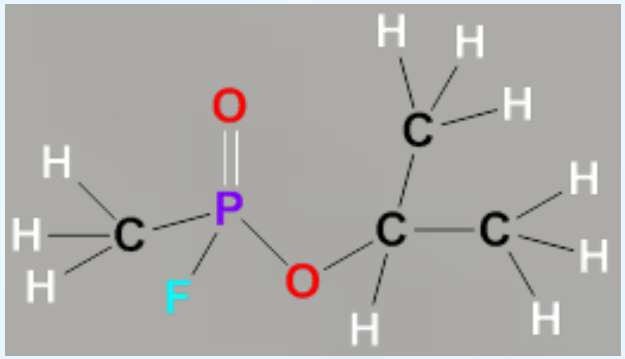
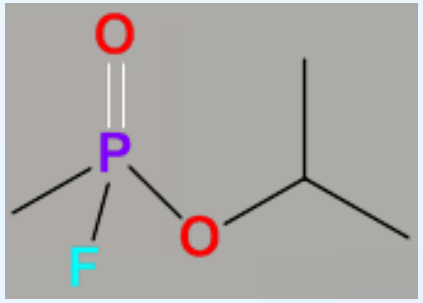
OPCW

Colour scheme of your model kit

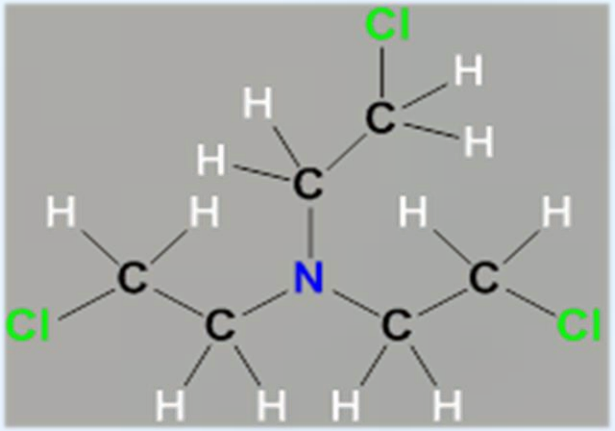
Molecular structure = Connected atoms

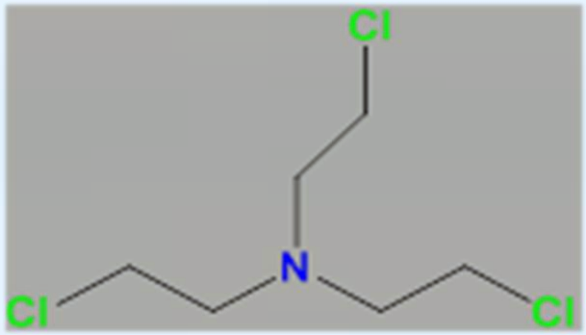
It's ok to be lazy and not use the letter "C" and not show the H atoms





Sarin





Nitrogen mustard (HN-3)

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Nitrogen (N)

Chorine (Cl)

Representation of che
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single (in grey) or doubl

Double bond

Single bond

Nitrogen mustard (HN-3)

Nitrogen mustard (HN-3)

Nitrogen mustard (HN-3)

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bonds are hidden,

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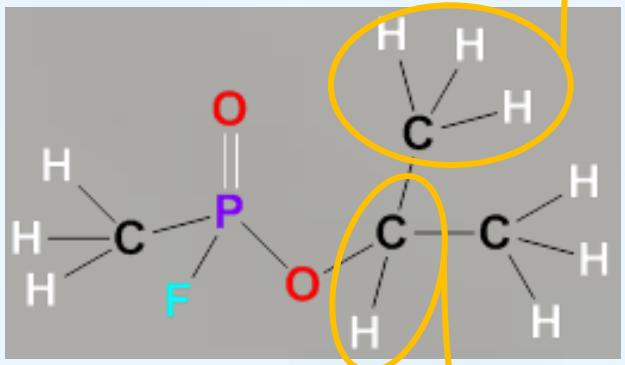

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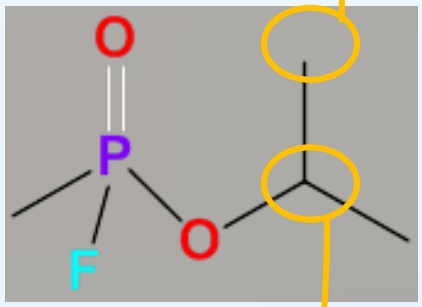

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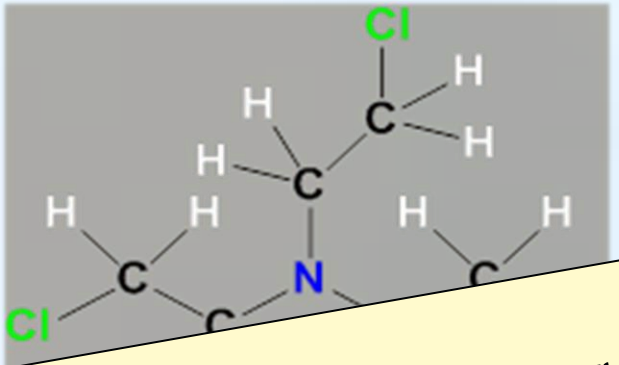
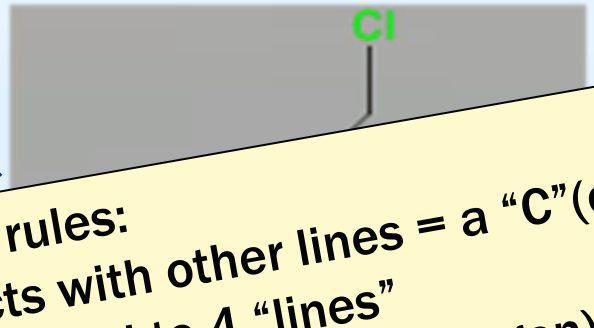




Double bond

Single bond

Nitrogen mustard

Nitrogen mustard (HN-3)

Nitrogen mustard (HN-3)

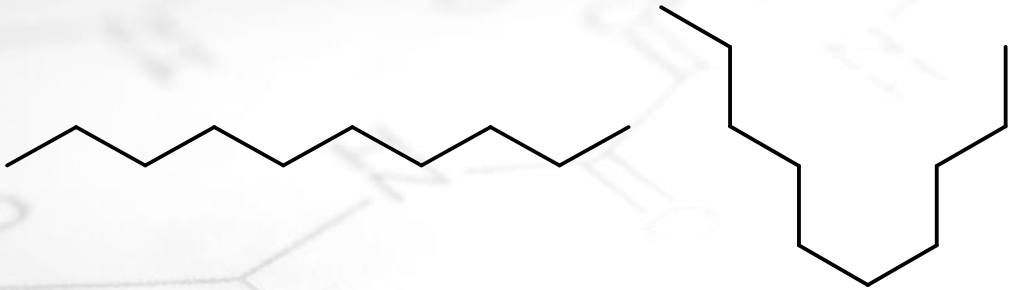
Simple rules:

Point where a line ends or intersects with other lines = a "C"(carbon)

"C" always is connected to 4 "lines"

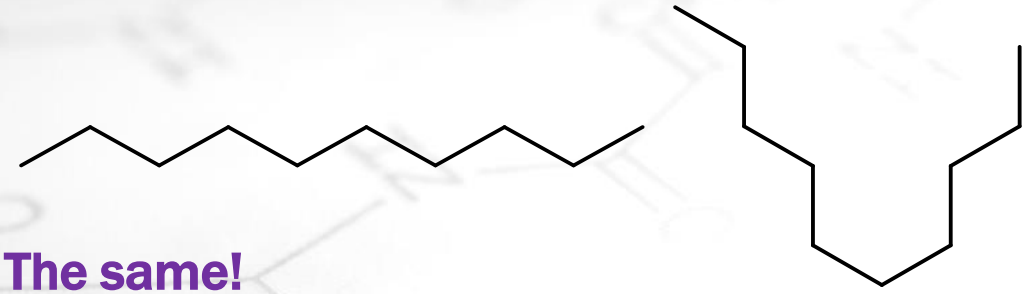
The missing lines are single bonds to "H" (hydrogen)

The Problem with Lazy...



The same or different?

The Problem with Lazy…

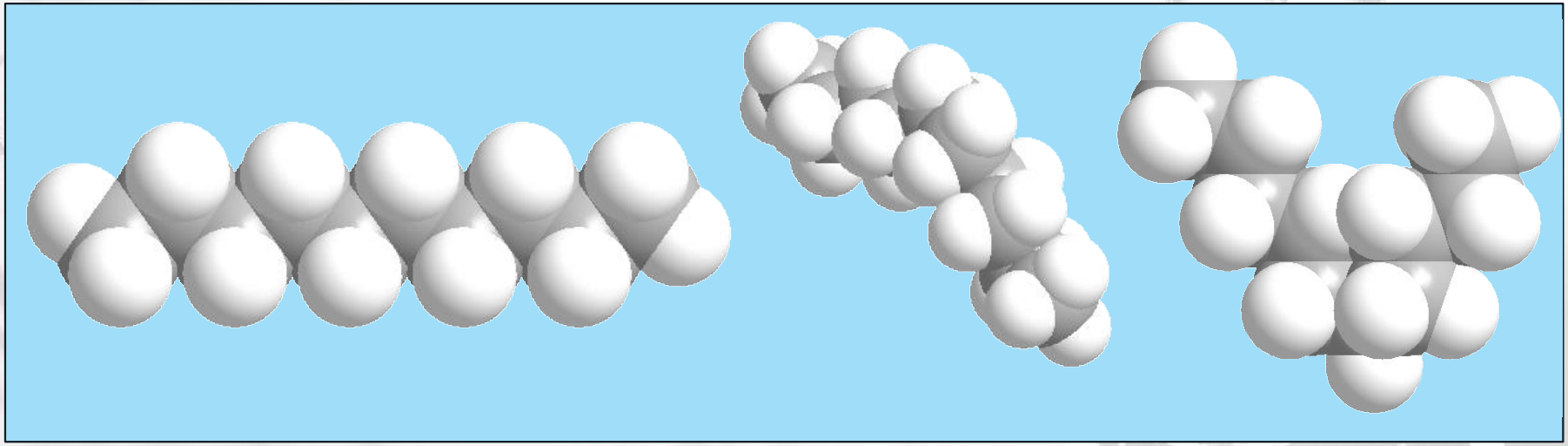


The same or different?

The same!

Both are C10 with identical connectivity between atoms

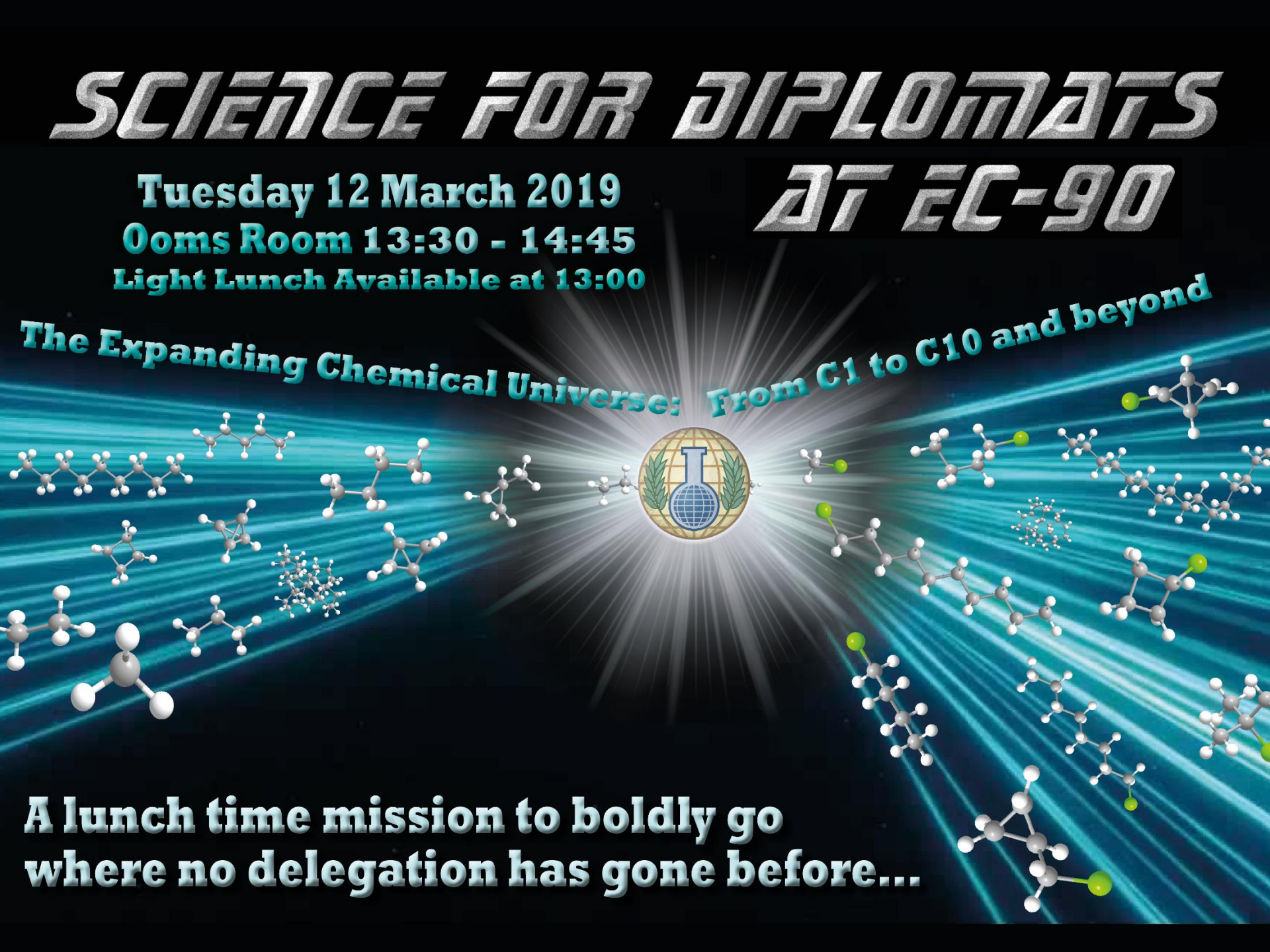
- Molecules are not “rigid” and can exist and be illustrated in a variety of configurations!



SCIENCE FOR DIPLOMATS AT EC-90

Tuesday 12 March 2019
Ooms Room 13:30 - 14:45
Light Lunch Available at 13:00

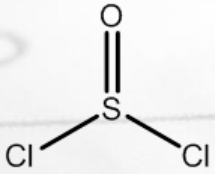
The Expanding Chemical Universe: From C1 to C10 and beyond



A lunch time mission to boldly go where no delegation has gone before…

Understanding Scheduled Chemicals

- **Example of a Specific Chemical: Schedule 3B.14**



Thionyl chloride

CAS 7719-09-7

Chemical name: Thionyl chloride

Schedule: 3B14

CAS RN: 7719-09-7 HS code: 2812.17

Key: 7719-09-7

Molecular formula: Cl2OS

CAS Index Name: Thionyl chloride

IUPAC name: Thionyl dichloride

Synonyms: UN1836

Thionyl chloride (SOCl2)

Sulfurous oxychloride

Sulfurous dichloride

Sulfur oxychloride (SOCl2)

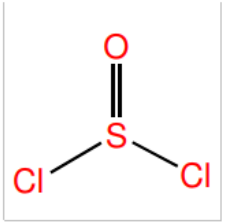
Sulfur oxychloride

Sulfur chloride oxide (SCl2O)

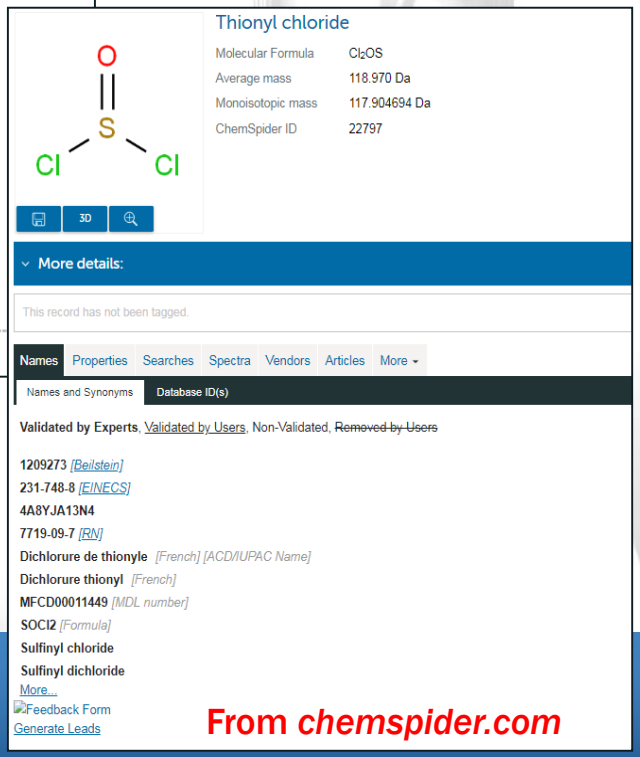
Sulfur chloride oxide (Cl2SO)

Sulfinyl dichloride

Sulfinyl chloride



From *OPCW Handbook on Chemicals*



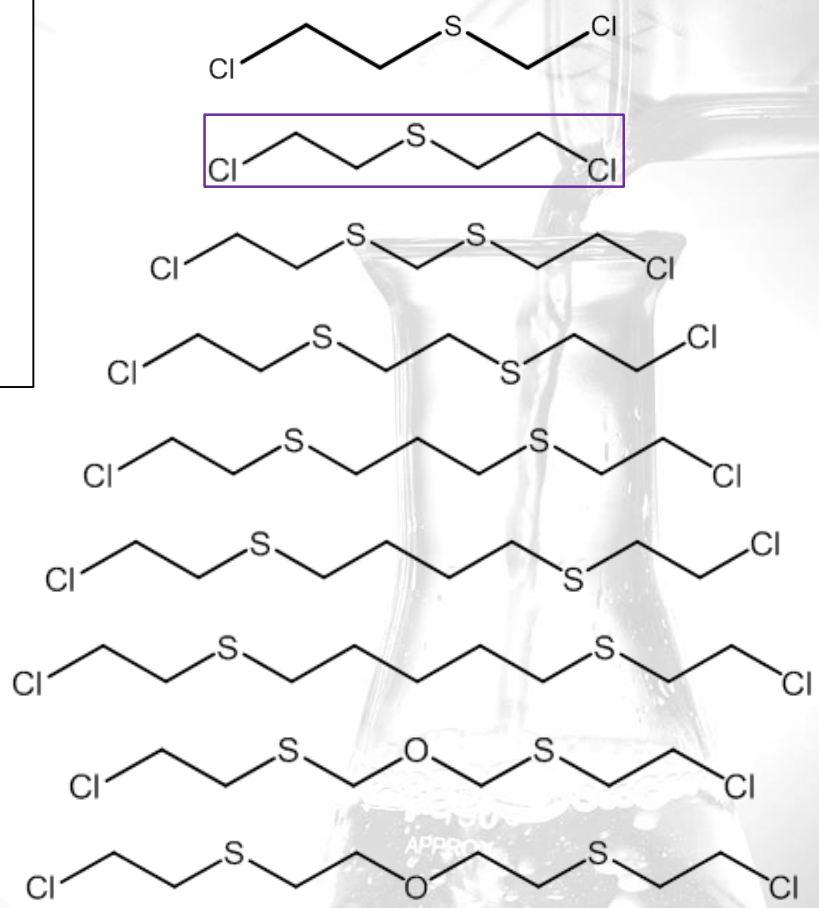
From *chemspider.com*

OPCW

Understanding Scheduled Chemicals

- **Example of a Group of Related Chemicals: Schedule 1A.04**

Sulfur mustards:	
2-Chloroethylchloromethylsulfide	(2625-76-5)
Mustard gas: Bis(2-chloroethyl)sulfide	(505-60-2)
Bis(2-chloroethylthio)methane	(63869-13-6)
Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane	(3563-36-8)
1,3-Bis(2-chloroethylthio)-n-propane	(63905-10-2)
1,4-Bis(2-chloroethylthio)-n-butane	(142868-93-7)
1,5-Bis(2-chloroethylthio)-n-pentane	(142868-94-8)
Bis(2-chloroethylthiomethyl)ether	(63918-90-1)
O-Mustard: Bis(2-chloroethylthioethyl)ether	(63918-89-8)



OPCW

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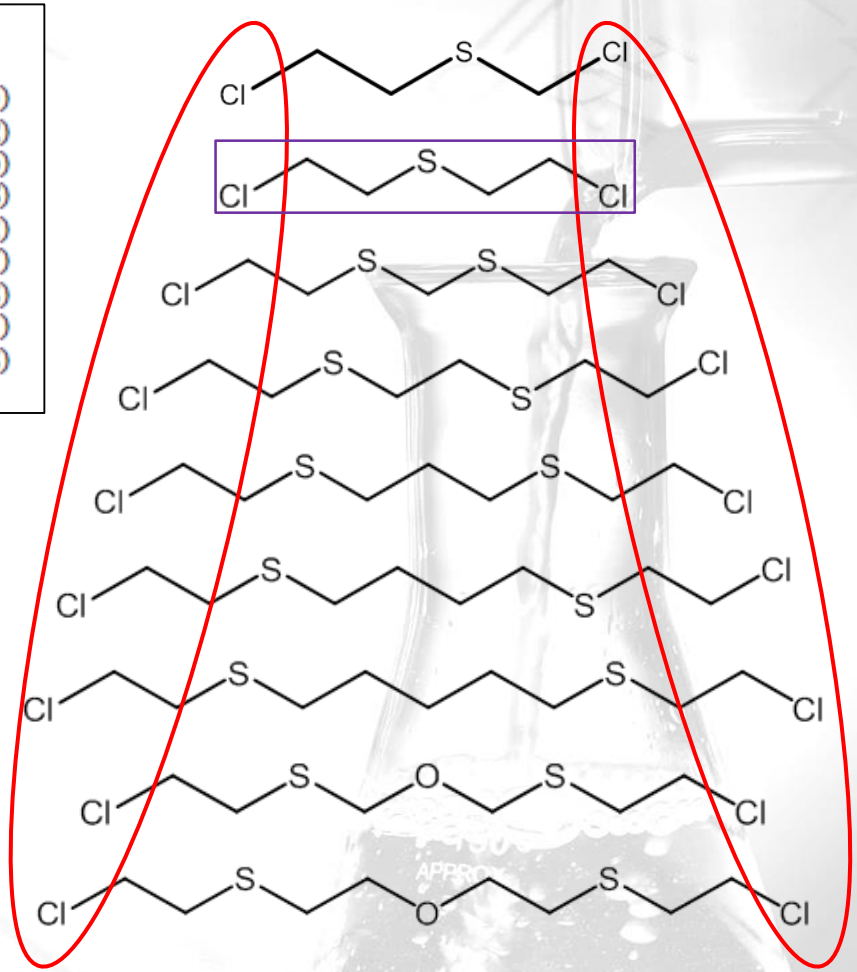

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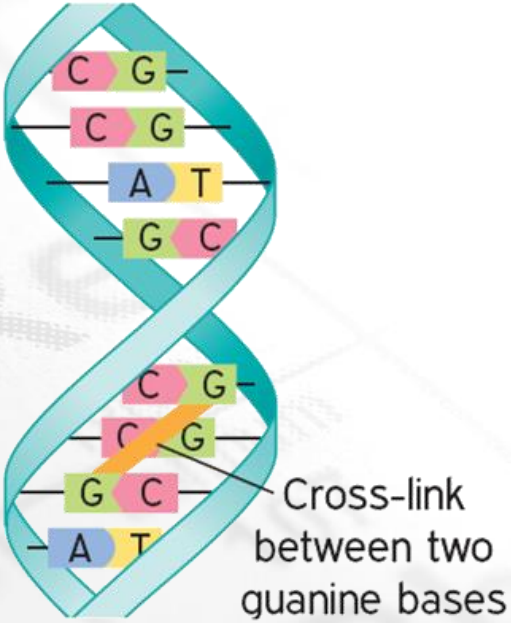

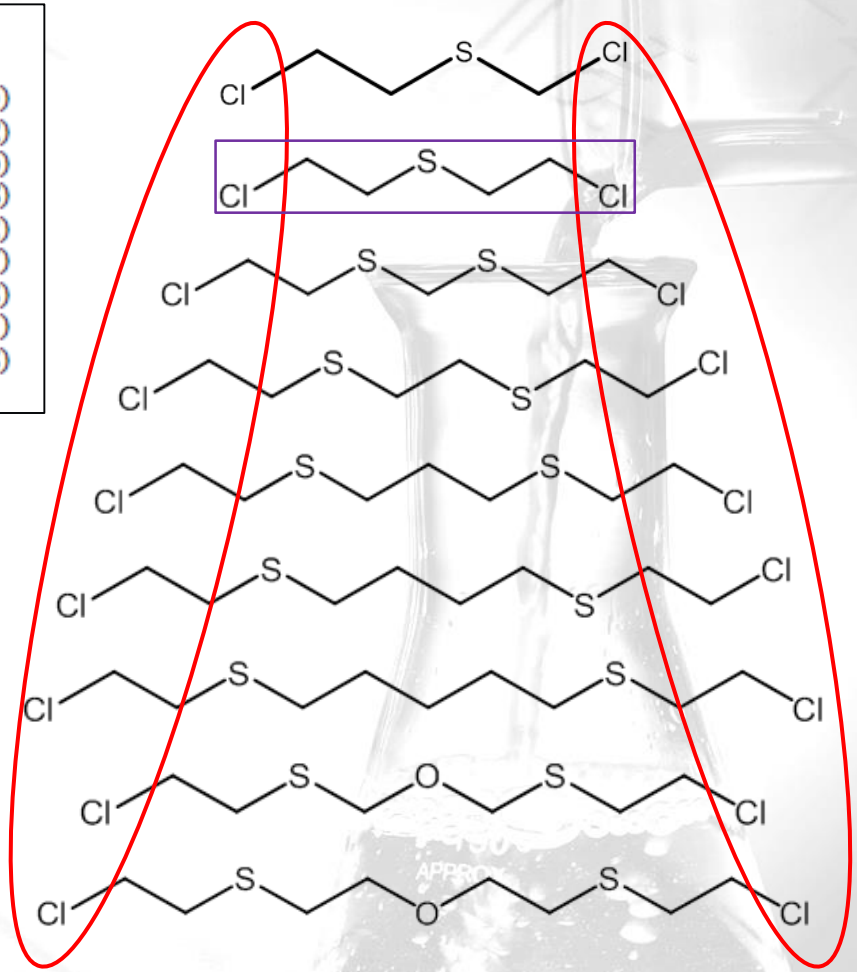

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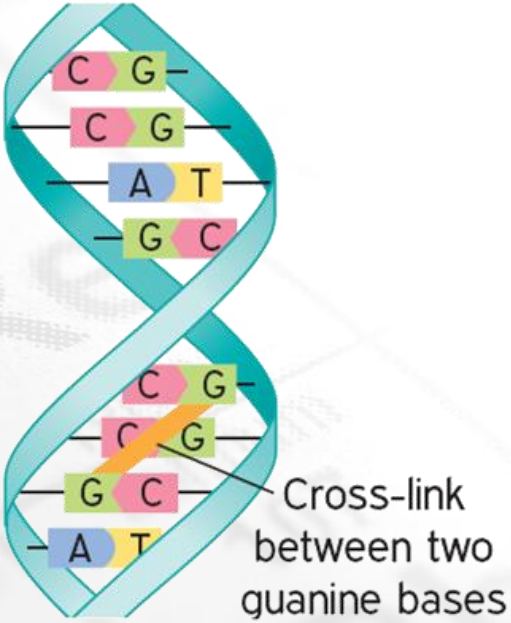

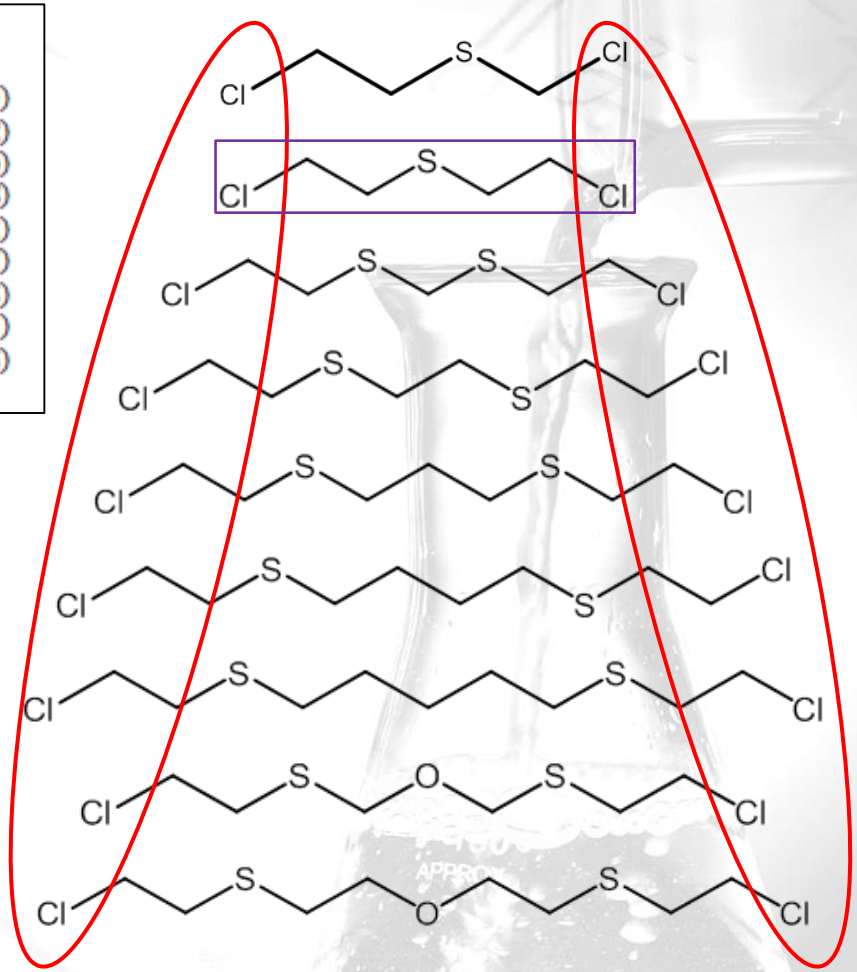

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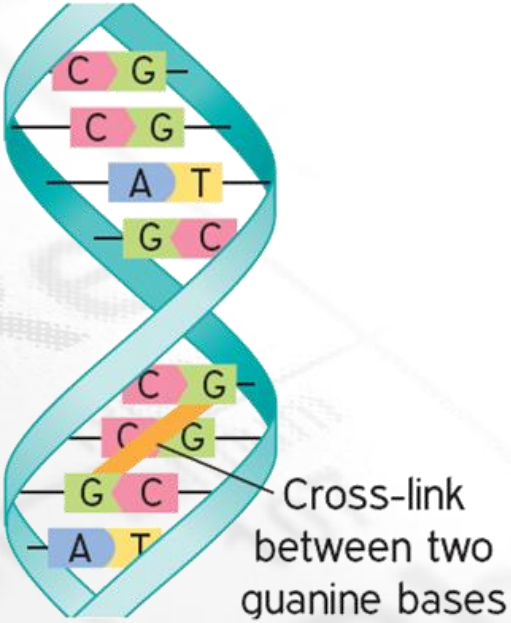
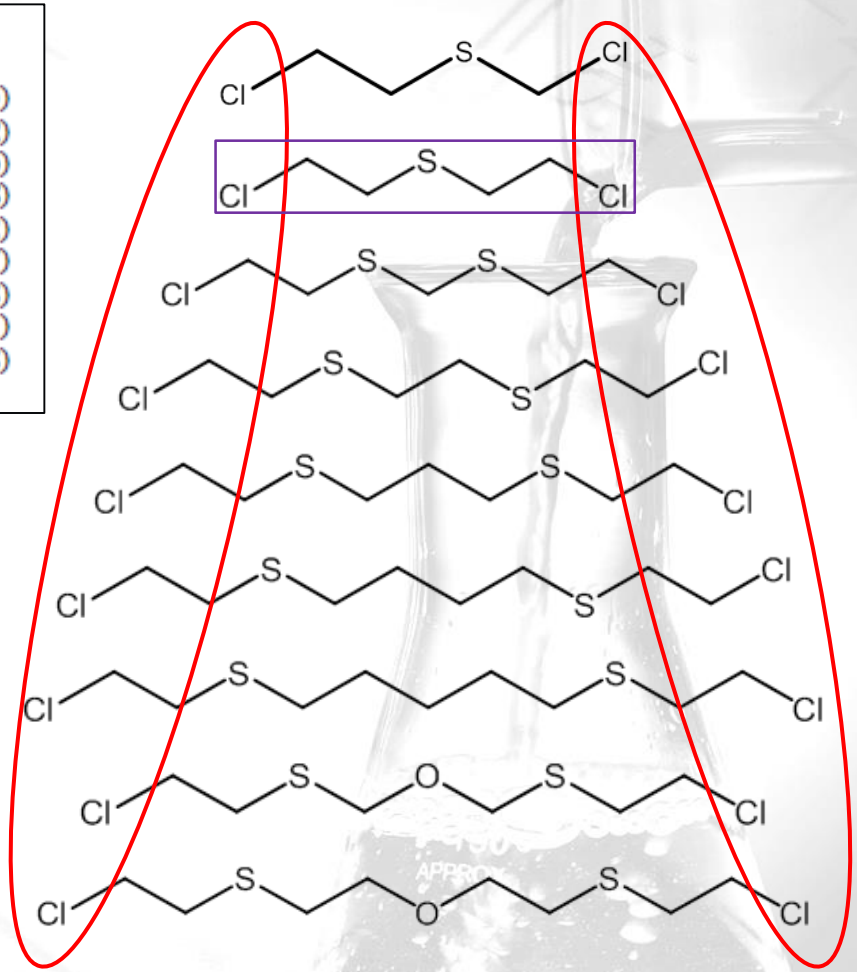
O-Mustard: Bis(2-chloroethylthioethyl)ether	(63918-89-8)





What About Families?

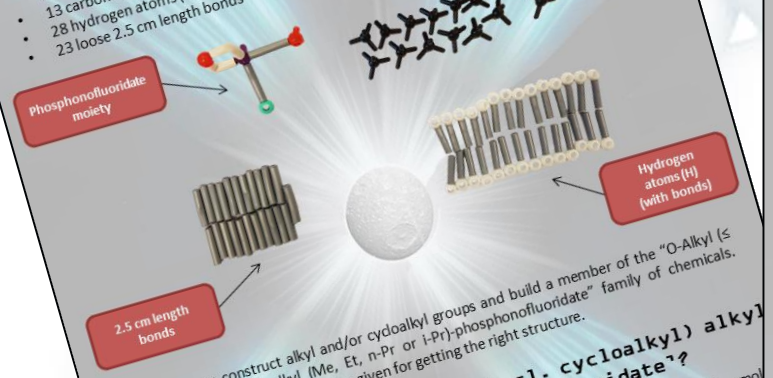
Expand your Chemical Universe
Construct a Molecule!

You are in posession of the "O-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates" Construction Kit

Instructions:

Your kit contains:

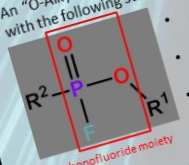
- 1 phosphonofluoridate moiety. This is a phosphorus center (P) bonded to two oxygen atoms (O) and one fluorine atom (F)
- 13 carbon atoms (C) without bonds
- 28 hydrogen atoms (H), each attached to a 2 cm length bonds
- 23 loose 2.5 cm length bonds



Your task is to construct alkyl and/or cycloalkyl groups and build a member of the "O-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" family of chemicals. Points will be rewarded and prizes given for getting the right structure.

What is an "O-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate"?

An "O-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" is a mol with the following structural features:



- A phosphonatefluoridate moiety as the core of the structure
- two alkyl groups; R^1 and R^2
- R^1 = any alkyl/cycloalkyl group from 1 to 10 C atoms in size attached to the P atom through a bridging O atom
- R^2 = Methyl (Me), Ethyl (Et), Isopropyl (i-Pr) or n-propyl (n-Pr) (these are specific alkyl groups of 1, 2 or 3 C atoms in size) attached directly to the P atom

Construct a Molecule
Score Sheet

Name: _____

Delegation: _____

Your task is to construct a member of the "O-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" family of chemicals. To do so, you must construct alkyl and/or cycloalkyl groups and attach them to the two free pegs of the O and P atoms of the phosphonofluoridate moiety. Following the rules outlined in the instruction handout, points will be rewarded based on the type of structures assembled for each group, as shown on the score sheet. Prizes will be given for those with the highest scores and for getting the structures right.

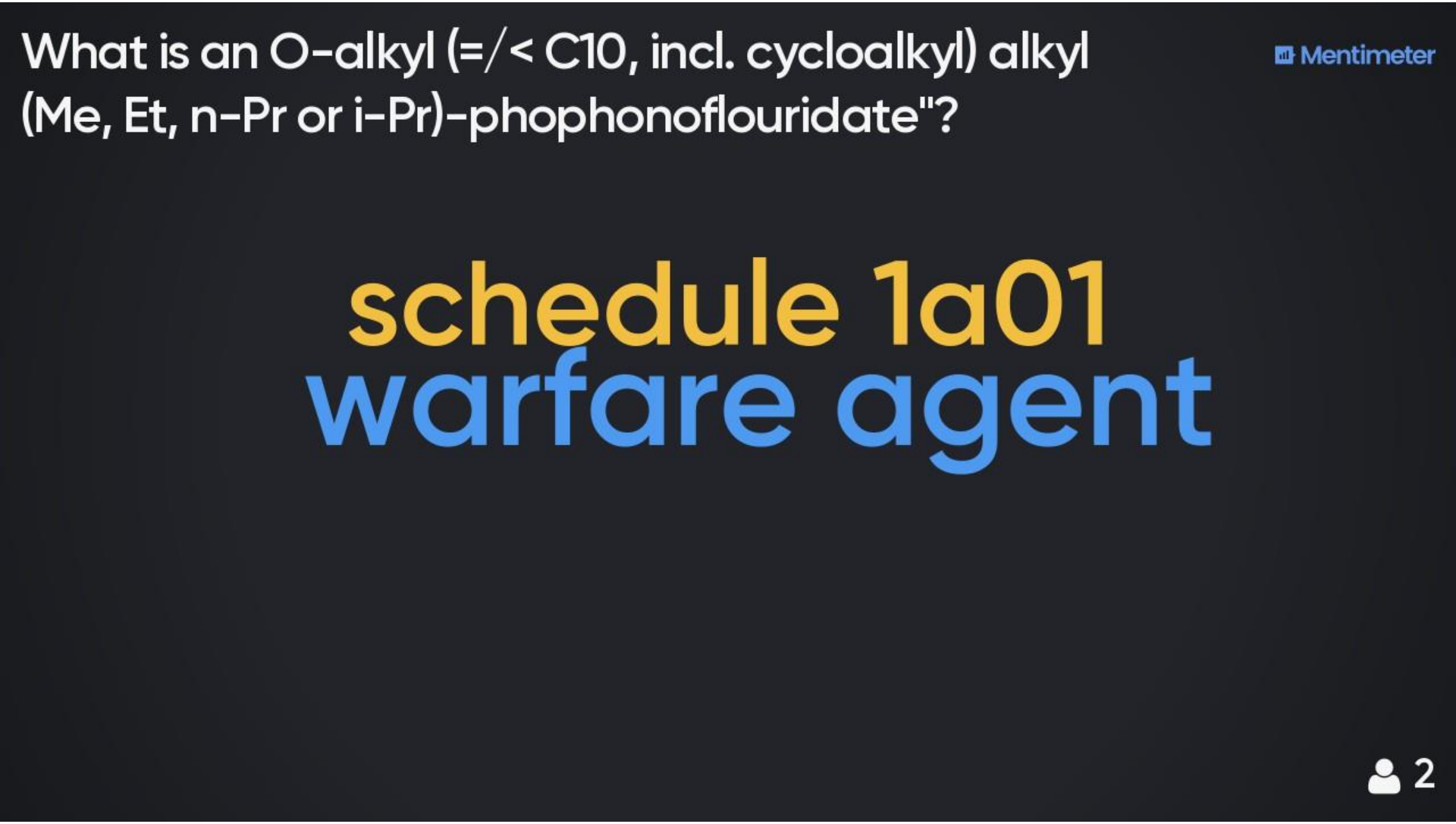
Score Sheet

	Chemical Structure	Points	Your Score
Beginner Level	Linear chain of carbon atoms	1	
	Branched chain of carbon atoms	+1	
Intermediate Level	Cyclic (a ring)	+1 (per ring)	
	Fused ring	+2	
Expert Level	Tertiary carbon atom	+2 (per C atom)	
	Quaternary carbon atom	+2 (per C atom)	
	Bicyclic	+3	
			Total:

What is an "O - Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate"?

OPCW

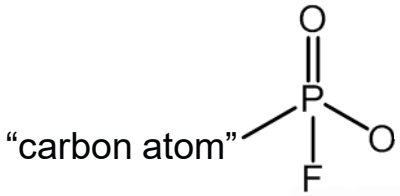
Answers from Participants

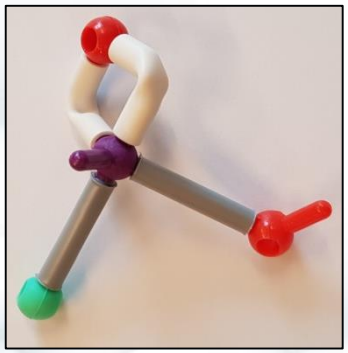


“*O*-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr) phosphonofluoridate”

C (alkyl group #1) B (alkyl group #2) A

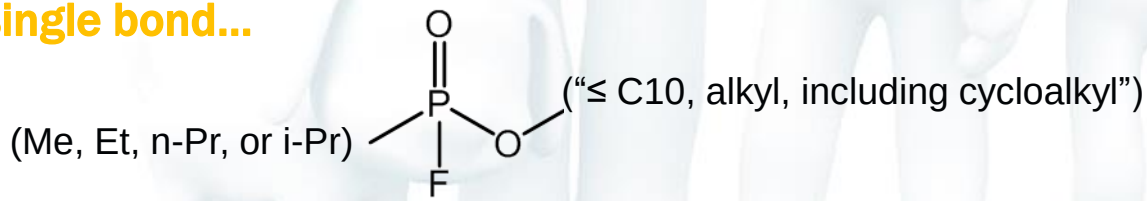
A: “phosphonofluoridate”



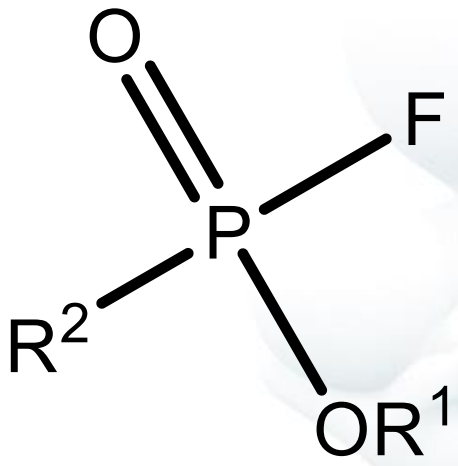


B: the “carbon atom” is part of an alkyl group… which is Me, Et, n-Pr or i-Pr

C: There is one other alkyl group : “≤ C10, incl. cycloalkyl” attached to the “O” with the single bond…



There is an Easier Way…



$R^1 \leq C_{10}$ alkyl, including cycloalkyl

R^2 = Me, Et, n-Pr, i-Pr

R = "the rest of the molecule" (a "moiety")

Me, Et, i-Pr, n-Pr and aklyl/cycloalkyl…
Do you know what to do?

“Alkyl” is a Substructure of an “Alkane”

- **An alkane is a molecule that is composed of carbon (C) and hydrogen (H) atoms**
  - Each carbon atom has four single bonds – to four other atoms (can be carbon or hydrogen)
  - Each hydrogen atom has one single bond to a carbon atom
- **Alkanes are a type of hydrocarbon**

PART IX (Verification Annex)

ACTIVITIES NOT PROHIBITED UNDER THIS CONVENTION IN ACCORDANCE WITH ARTICLE VI

REGIME FOR OTHER CHEMICAL PRODUCTION FACILITIES

A. DECLARATIONS

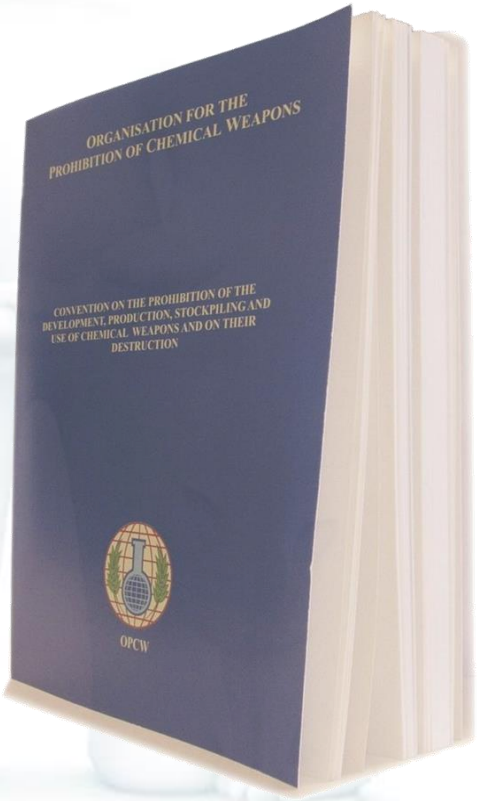
List of other chemical production facilities

1. The initial declaration to be provided by each State Party pursuant to Article VI, paragraph 7, shall include a list of all plant sites that:

   (a) Produced by synthesis during the previous calendar year more than 200 tonnes of unscheduled discrete organic chemicals; or

   (b) Comprise one or more plants which produced by synthesis during the previous calendar year more than 30 tonnes of an unscheduled discrete organic chemical containing the elements phosphorus, sulfur or fluorine (hereinafter referred to as "PSF-plants" and "PSF-chemical").

2. The list of other chemical production facilities to be submitted pursuant to paragraph 1 shall not include plant sites that exclusively produced explosives or hydrocarbons.



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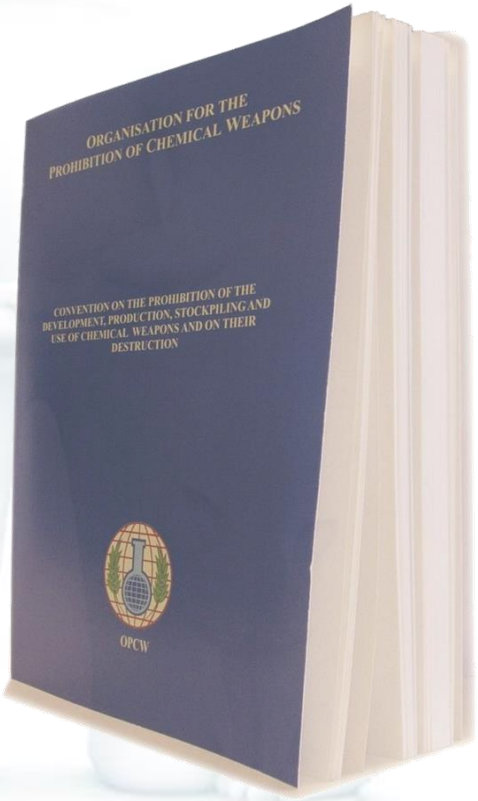
2. The list of other chemical production facilities to be submitted pursuant to paragraph 1 shall not include plant sites that exclusively produced explosives or hydrocarbons.

Please build a 1 carbon alkane (no declaration required)

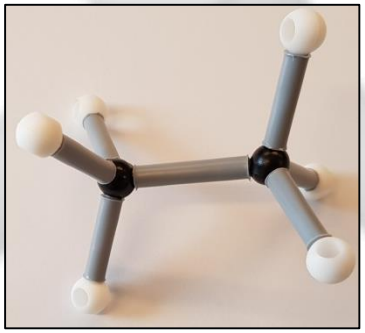


From C1 to C3…

- Does your C1 Alkane look like this?

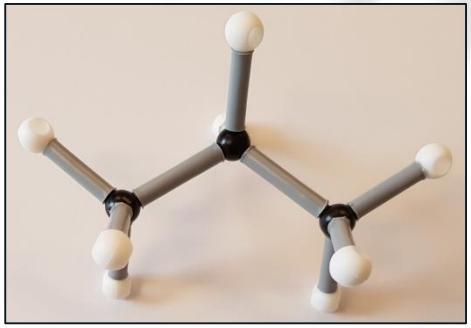
Methane, CH_4

- Now build a C2 alkane



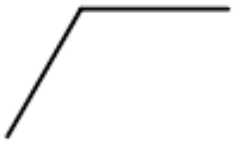
Ethane, C_2H_6

- And finally, build a C3 alkane



Propane, C_3H_8

=



From C1 to C3…

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Methane, CH_4

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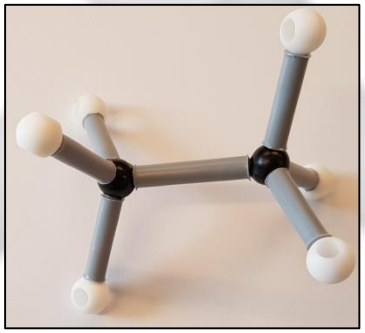
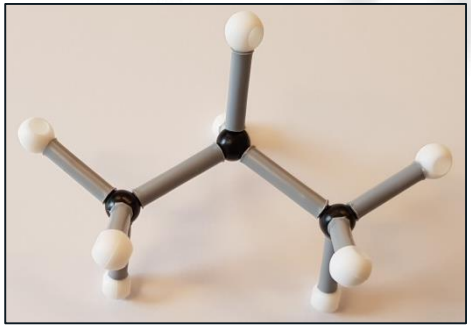


Ethane, C_2H_6

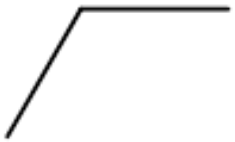
Did anyone build one of these?

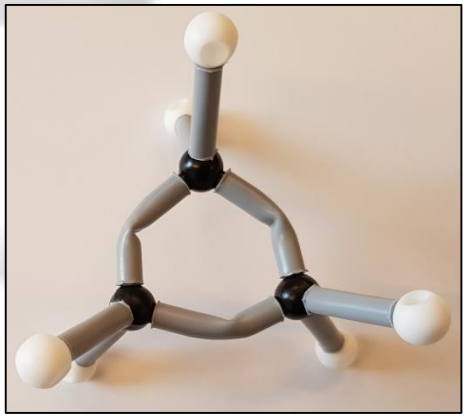
- And finally, build a C3 alkane



Propane, C_3H_8

=





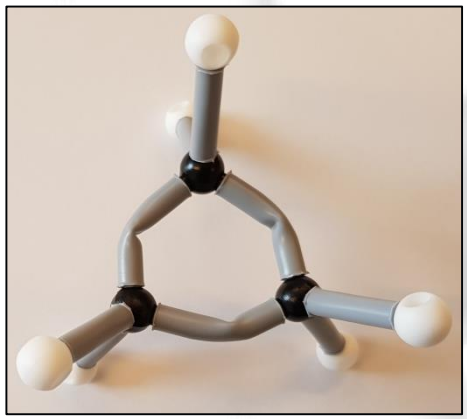
Cyclopropane

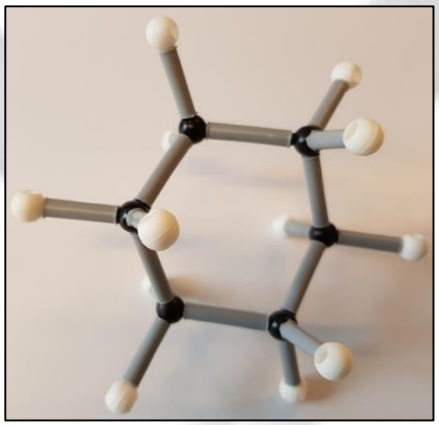
C_3H_6

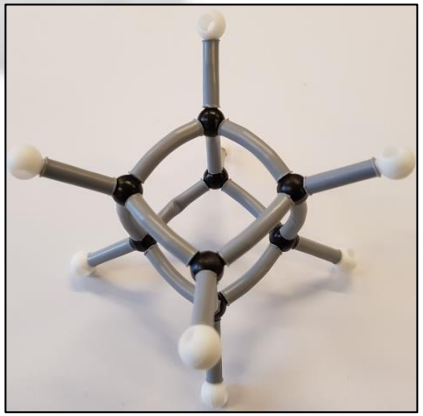
The smallest "cycloalkane"

Cycloalkanes

"Cubane"







"Strained Bonds"

Six-membered ring allows for more optimal bonding geometry

Still ways to strain larger cycloalkanes!

Cycloalkanes

CAS Registry Number: 13172-14-0
Formula: $C_7 H_{12} F O_2 P$
CA Index Name: Phosphonofluoridic acid, methyl-, bicyclo[2.2.0]hex-2-yl ester (7CI,8CI)

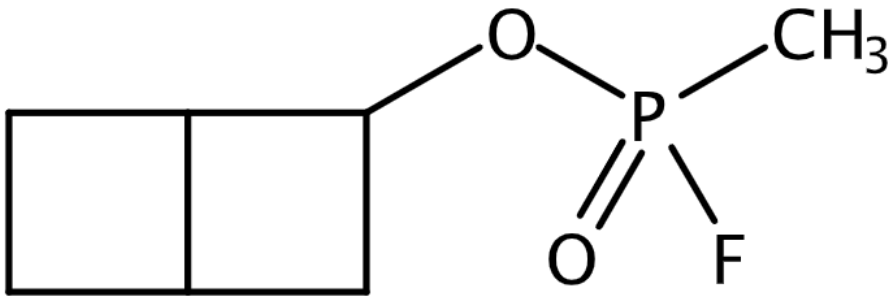
Other Names
Bicyclo[2.2.0]hexan-2-ol, methylphosphonofluoridate

Number of References
~1

Document Types
Journal

Properties
Predicted

Commercial Sources
Not Available



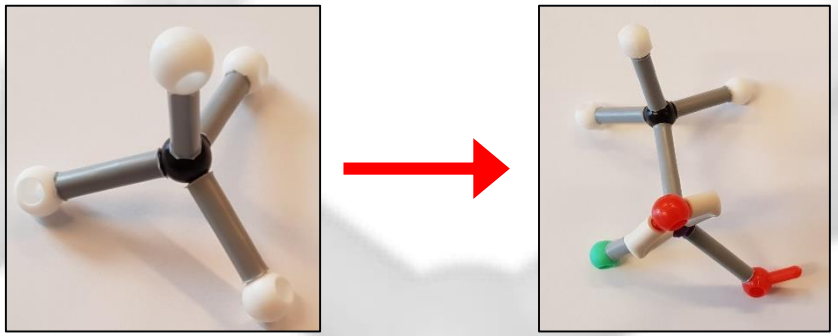
All connections that meet the "rules" for an alkane are allowed!
(and some strained molecules may be unstable)

From “Alkanes” to “Alkyls”

- Remove one hydrogen atom (and the short bond to which is attached)
- Attach the “alkyl group” to another molecular structure through one of the free bonds in your kit!

From Methane to “Methyl”

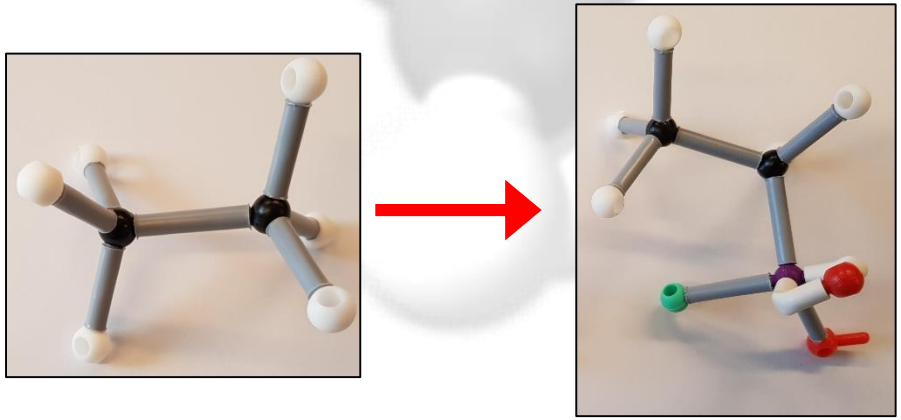
CH_4 to CH_3X



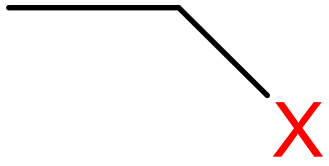
“Me”

From Ethane to “Ethyl”

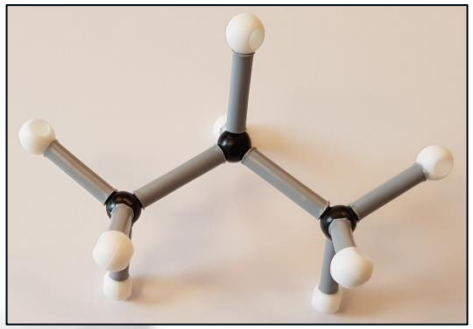
C_2H_6 to CH_3CH_2X

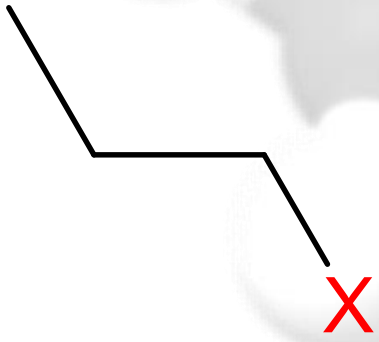


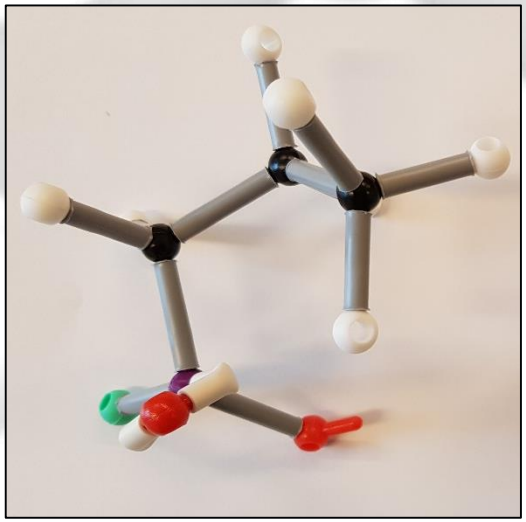
“Et”

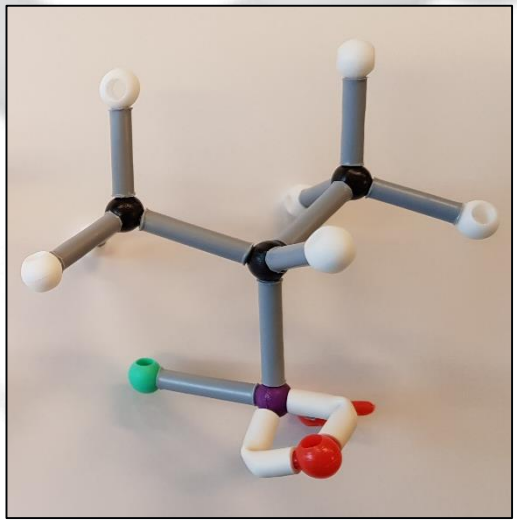


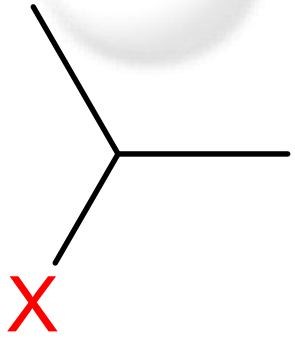
What About Propane?











2 Isomers: “n-Pr” “i-Pr”

Significance of Carbon Atoms: Additional Molecular Possibilities

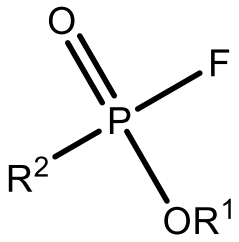
Number of Alkyl Carbon Atoms	Parent Alkane Structures	Alkyl Group Structures
C = 1	CH_4	$H_3C—X$ ("methyl" or "Me")
C = 2	$H_3C—CH_3$	H_3C (X) ("ethyl" or "Et")
C = 3	H_3C CH_3	H_3C (X) ("n-propyl" or "n-Pr"); H_3C ("iso-propyl" or "i-Pr") CH_3 (X)
C = 4	alkanes: H_3C CH_3; H_3C CH_3 H_3C	CH_3 (X); H_3C (X) CH_3; H_3C CH_3 (X); H_3C (X)
	a cycloalkane and an alkane with a cycle: CH_3	(X); CH_3 (X); (X)
	others ways to connect the carbon atoms	(X); CH_3 (X); (X)

R^2 alkyl groups!

OPCW

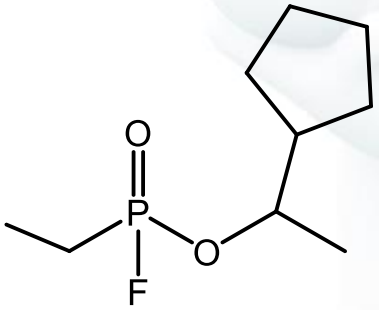
From C1 to C4:
10 Alkanes provide 15 possible alkyl groups
All possibilities allowed for R^1 from C1 to C10!

Are these "O - Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates"?



$R^1 \leq C_{10}$ alkyl, including cycloalkyl

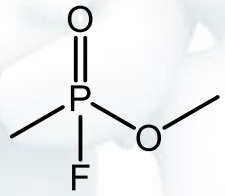
R^2 = Me, Et, n-Pr, i-Pr



R^1 = C7

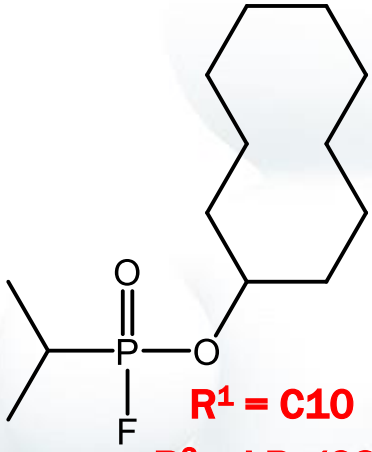
R^2 = Et (C2)

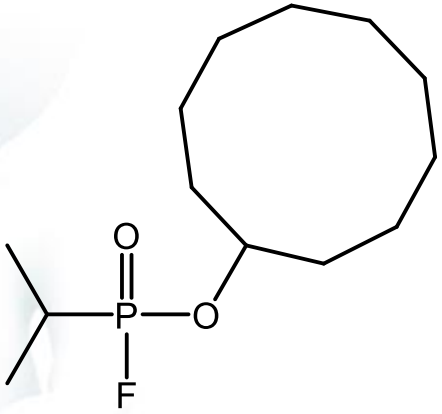
Yes



$R^1 = R^2$ = Me (C1)

Yes



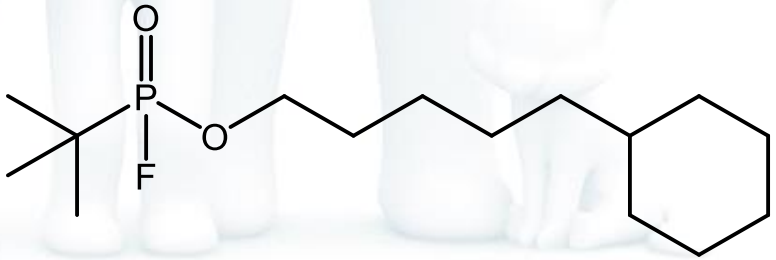


R^1 = C10

R^2 = i-Pr (C3)

Yes

(both are the same)



R^1 = C11

R^2 = C4

No

Your Turn to Explore "Chemical Space"

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Instructions:

Your kit contains:

- 1 phosphonofluoridate moiety. This is a phosphorus center (P ●) bonded to two oxygen atoms (O ●) and one fluorine atom (F ●)
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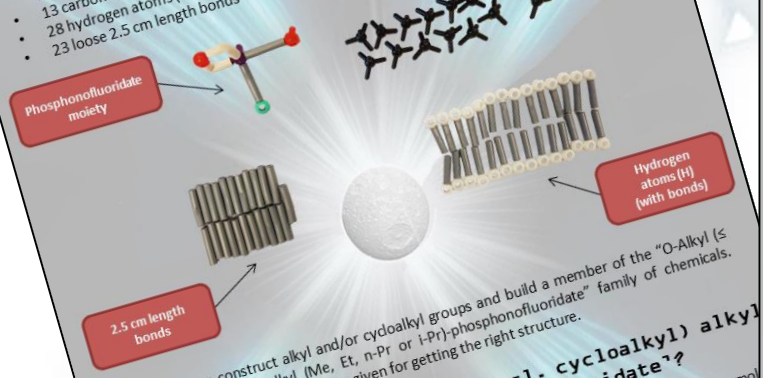

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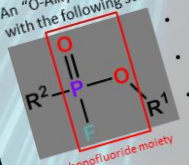

- A phosphonatefluoridate moiety as the core of the structure
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- R^1 = any alkyl/cycloalkyl group from 1 to 10 C atoms in size attached to the P atom through a bridging O atom
- R^2 = Methyl (Me), Ethyl (Et), Isopropyl (i-Pr) or n-propyl (n-Pr) (these are specific alkyl groups of 1, 2 or 3 C atoms in size) attached directly to the P atom

Construct a Molecule
Score Sheet

Name: _____

Delegation: _____

Your task is to construct a member of the "O-Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" family of chemicals. To do so, you must construct alkyl and/or cycloalkyl groups and attach them to the two free pegs of the O and P atoms of the phosphonofluoridate moiety. Following the rules outlined in the instruction handout, points will be rewarded based on the type of structures assembled for each group, as shown on the score sheet. Prizes will be given for those with the highest scores and for getting the structures right.

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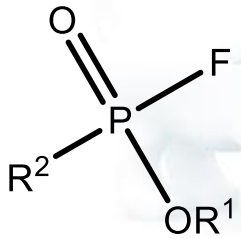
	Branched chain of carbon atoms	+1	
Intermediate Level	Cyclic (a ring)	+1 (per ring)	
	Fused ring	+2	
Expert Level	Tertiary carbon atom	+2 (per C atom)	
	Quaternary carbon atom	+2 (per C atom)	
	Bicyclic	+3	
			Total:

OPCW

How Many Ways Can the Carbon and Hydrogen Atoms be Arranged?

Carbon Atoms	Acyclic Isomers	Attachment Possibilities for R-X	Isomers with cycles	Attachment Possibilities for R-X	C1 to Cn Possibilities
1	1	1	0	0	**1**
2	1	1	0	0	**2**
3	1	2	1	1	**5**
4	2	4	4	7	**16**
5	3	8	10	39	**63**
6	5	17	26	84	**164**
7	9	39	71	374	**577**
8	18	89	?	?	**> 666**
9	35	211	?	?	**> 877**
10	75	507	?	?	**> 1384**

For C8 to C10 cycloalkyls: a computational study is required to find the possibilities!



> 1384 possible alkyl groups

R^1 ≤ C_{10} alkyl, including cycloalkyl

R^2 = Me, Et, n-Pr, i-Pr

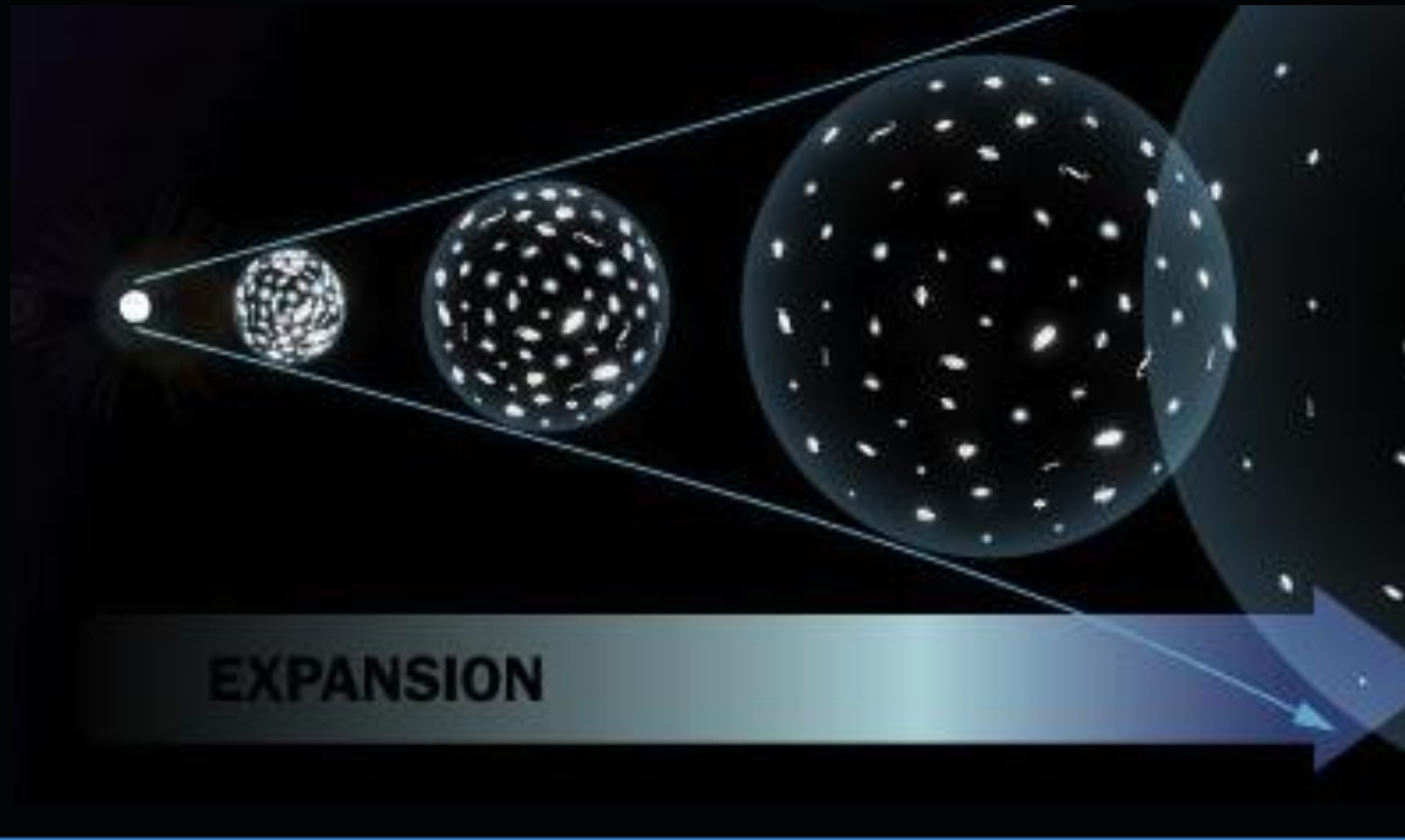
4 possible alkyl groups

> (4 X 1384 =) 5536

Schedule 1A.01

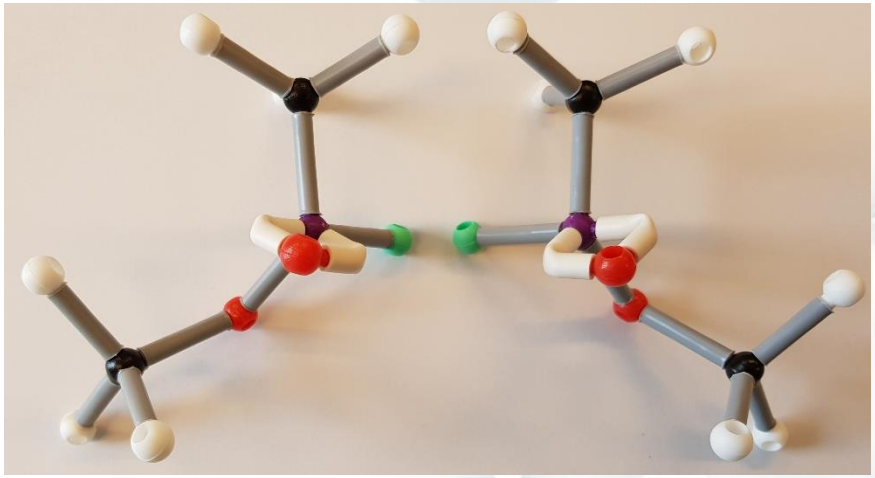
Parent Structures!

From C1 to Cn…

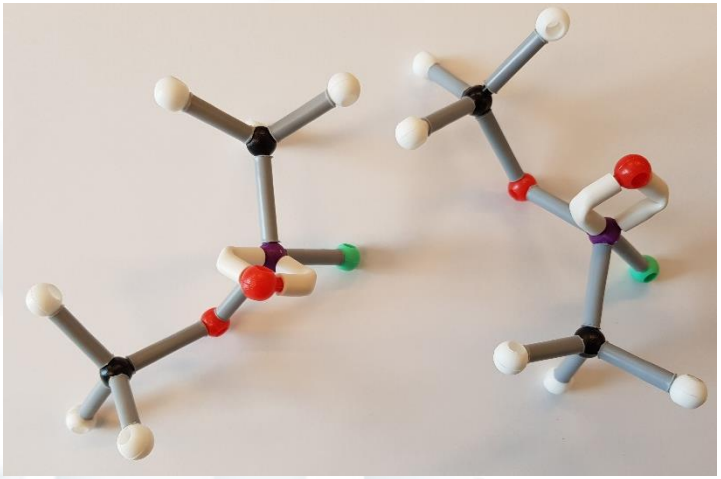


“Parent Structures” are Far From the Whole Story…

- **Molecules have 3-Dimensional Spatial Orientations**



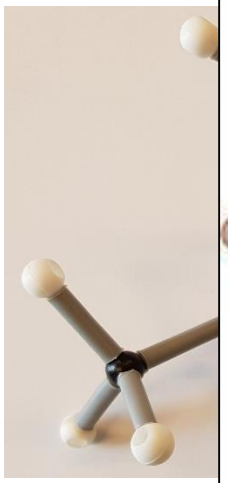
“Mirror images”

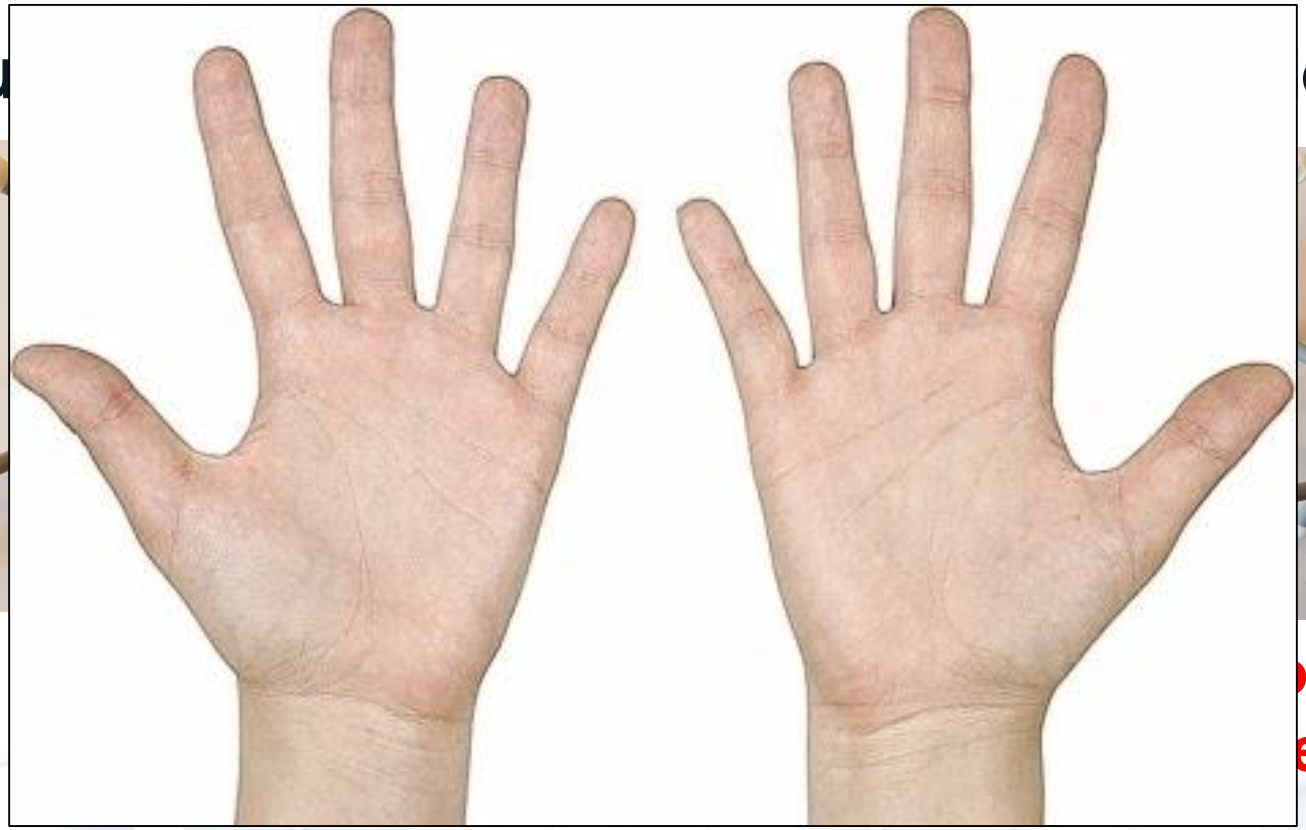


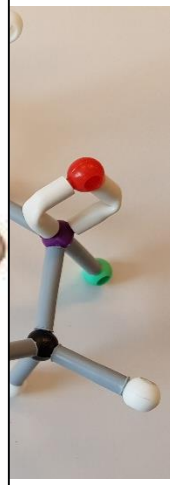
Cannot rotate and convert one for to the other!

“Parent Structures” are Far From the Whole Story…

- **Molecu** **ons**

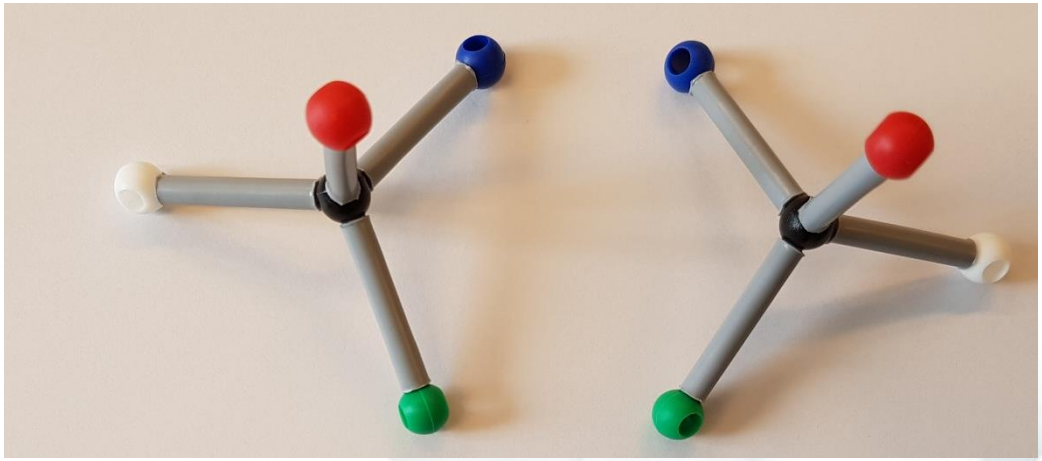




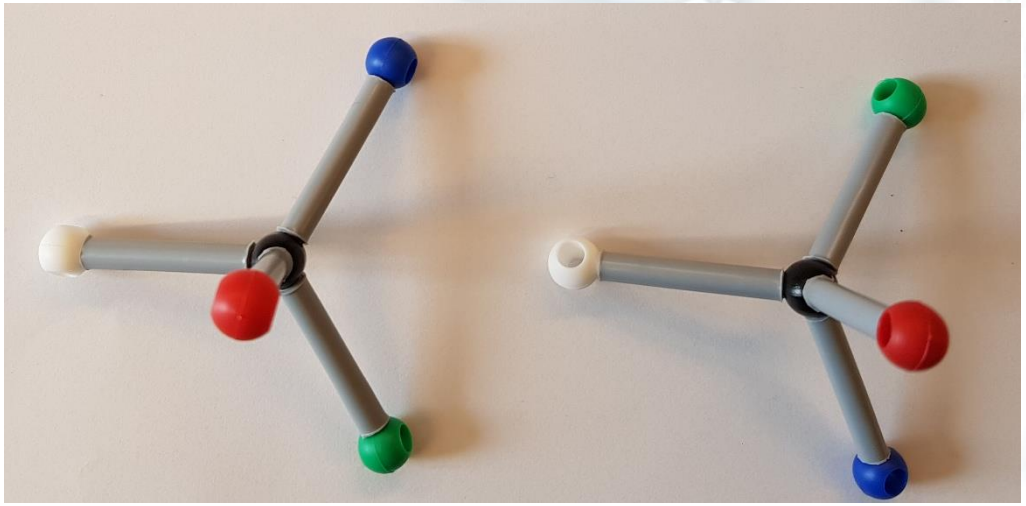


nvert
er!

Stereoisomers Occur Whenever an Atom has Four Non-Equivalent Connections ("Chirality")

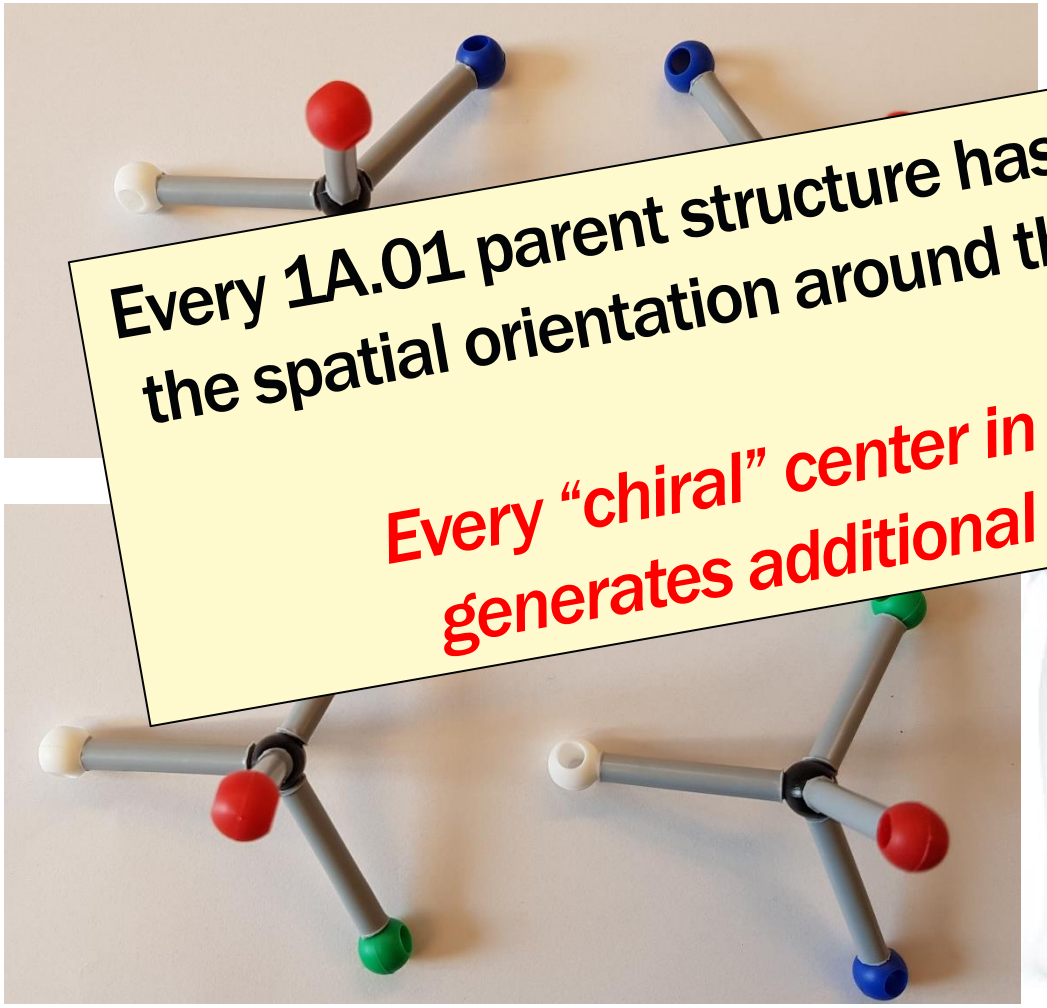


Mirror Images



Cannot rotate and convert one for to the other!

Stereoisomers Occur Whenever an Atom has Four Non-Equivalent Connections ("Chirality")

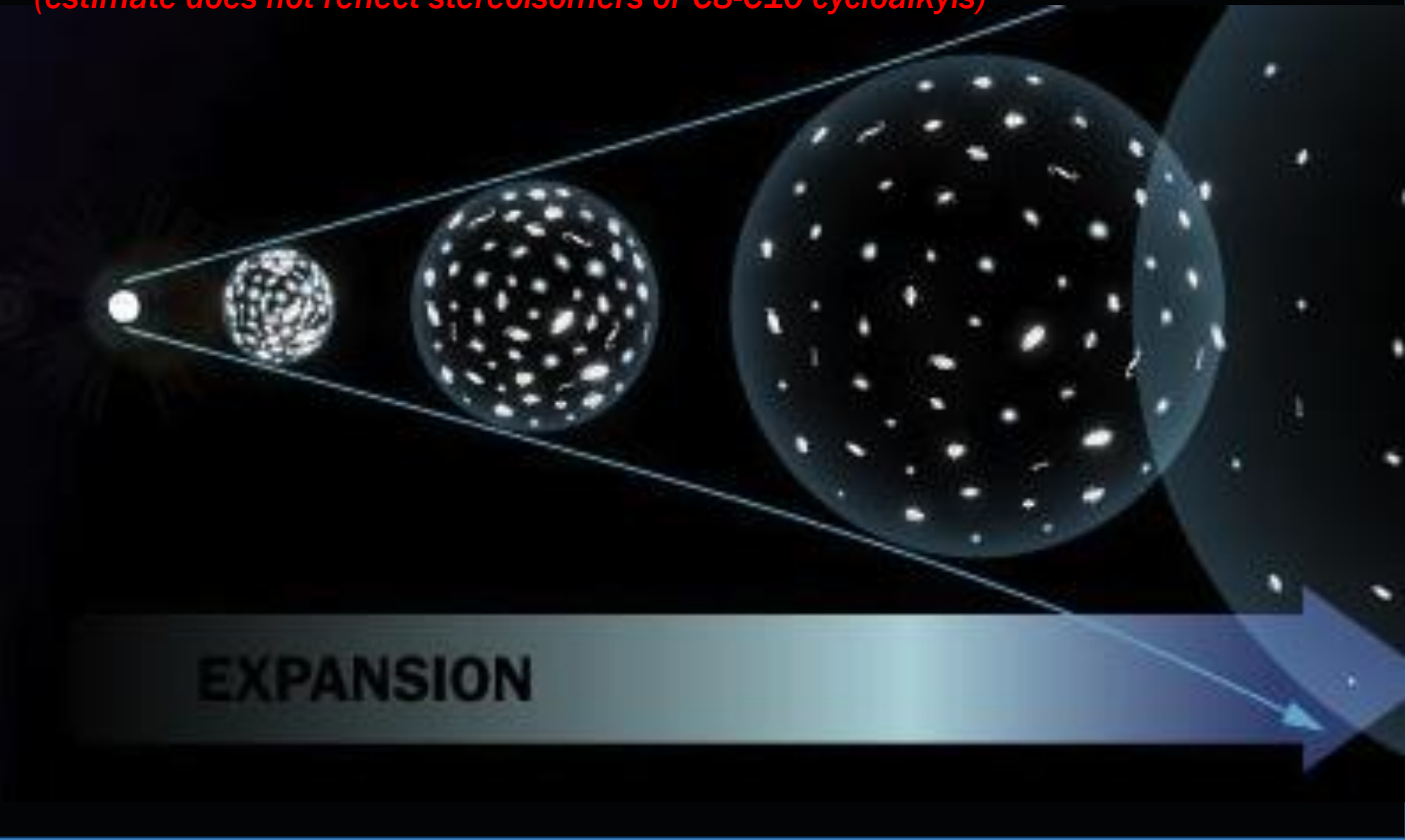


Every 1A.01 parent structure has 2 stereoisomers for the spatial orientation around the phosphorus atom

Every "chiral" center in an alkyl group generates additional steroisomers

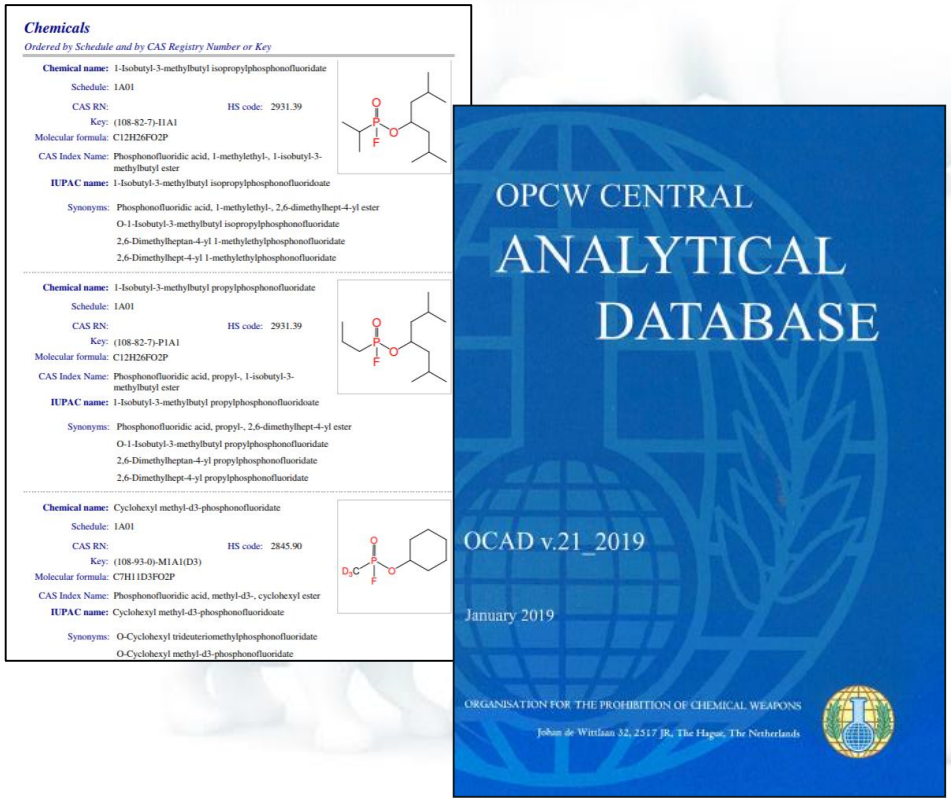
Cannot rotate and convert one for to the other!

From C1 to C10, >> 5536!
(estimate does not reflect stereoisomers or C8-C10 cycloalkyls)



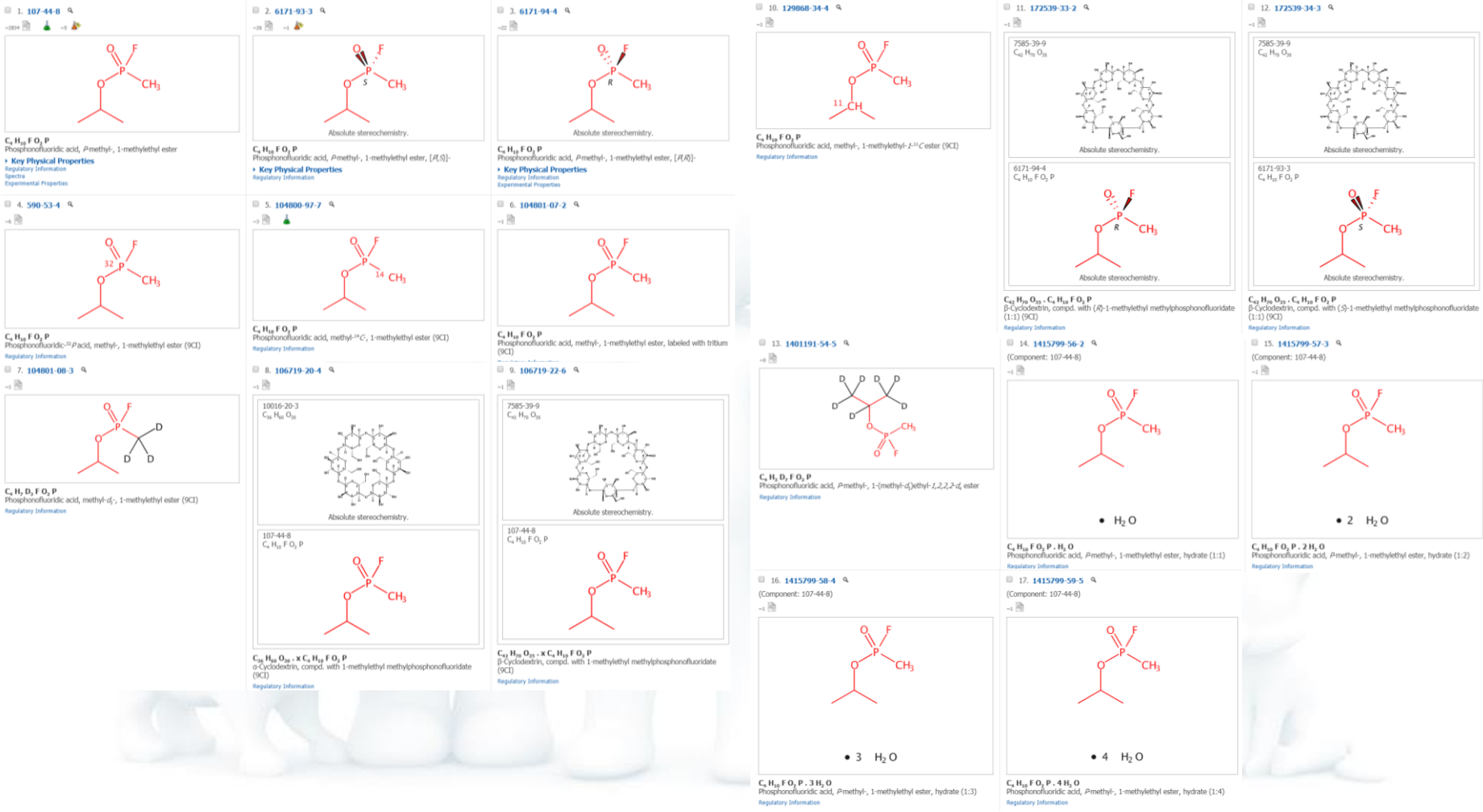
Thousands Possible, How Many Are Actually Known?

CAS®
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY



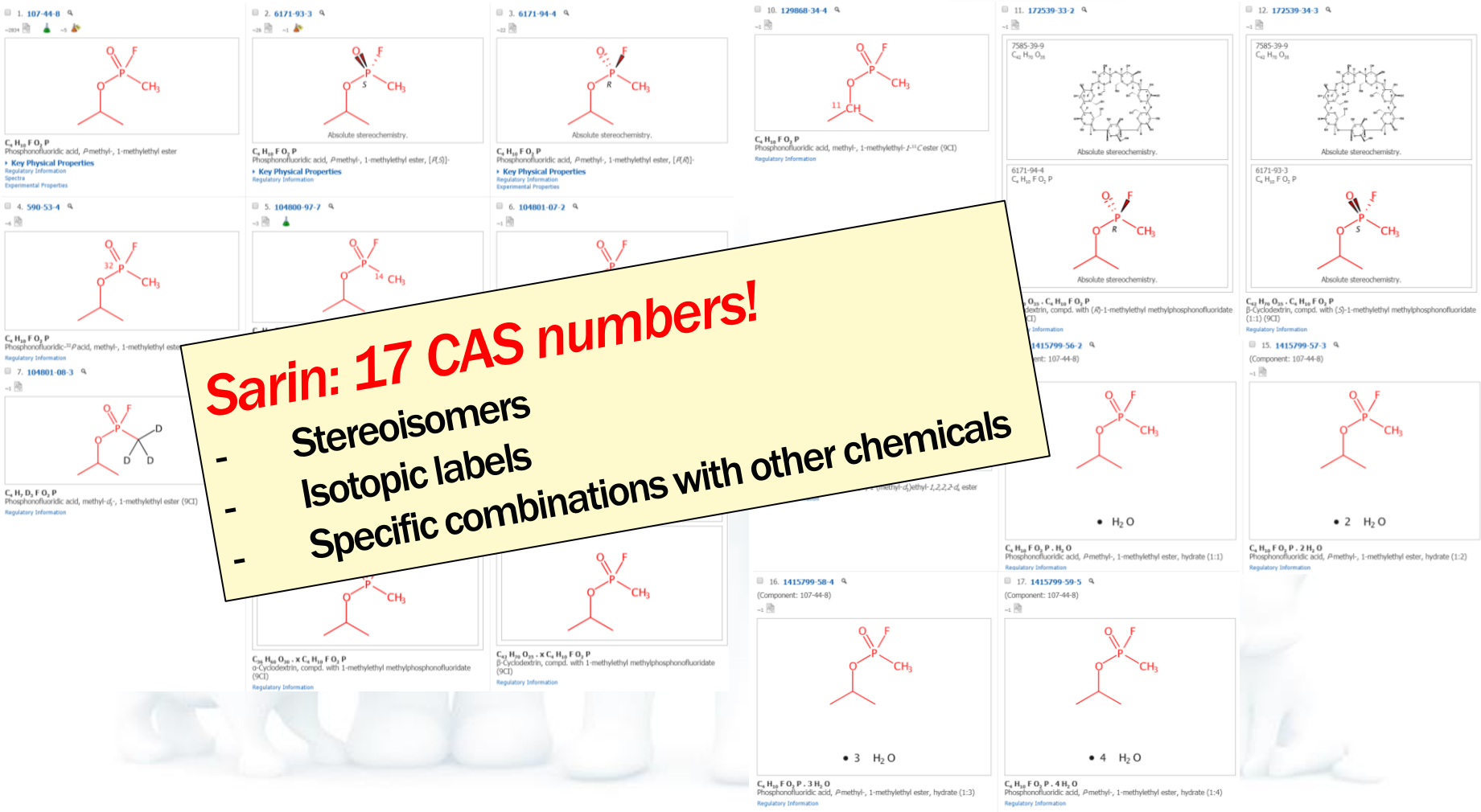
- **CAS Database: 472 1A.01 chemical substances**
- **OPCW handbook on chemicals: 376 1A.01 chemicals**
- **OCAD V21: 569 1A.01 Mass Spectra**

The Most Famous Member of the "O - Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" Family?



OPCW

The Most Famous Member of the "O - Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" Family?



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The Most Famous Member of the "O - Alkyl (≤ C10, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridate" Family?

DE GRUYTER

Pure Appl. Chem. 2018; aop

Conference paper

Christopher M. Timperley*, Jonathan E. Forman*, Mohammad Abdollahi, Abdullah Saeed Al-Amri, Isel Pascual Alonso, Augustin Baulig, Veronica Borrett, Flerida A. Cariño, Christophe Curty, David Gonzalez, Zrinka Kovarik, Roberto Martínez-Álvarez, Robert Mikulak, Nicia Maria Fusaro Mourão, Ponnadurai Ramasami, Slawomir Neffe, Syed K. Raza, Valentin Rubaylo, Koji Takeuchi, Cheng Tang, Ferruccio Trifirò, Francois Mauritz van Straten, Paula S. Vanninen, Volodymyr Zaitsev, Farhat Waqar, Mongia Saïd Zina, Stian Holen and Hope A. Weinstein

Advice from the Scientific Advisory Board of the Organisation for the Prohibition of Chemical Weapons on isotopically labelled chemicals and stereoisomers in relation to the Chemical Weapons Convention

https://doi.org/10.1515/pac-2018-0803

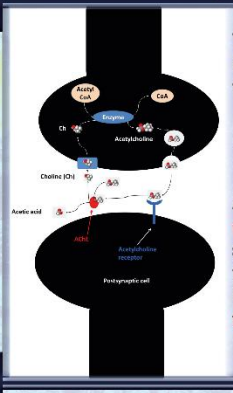
Article note: A special issue containing invited papers on Innovative Technologies for Chemical Security, based on work done within the framework of the Chemical Weapons Convention.

OPCW

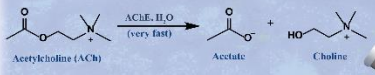
Acetylcholinesterase Inhibition

created by Sofía Sola Sancho and Maria Hemme

Acetylcholinesterase



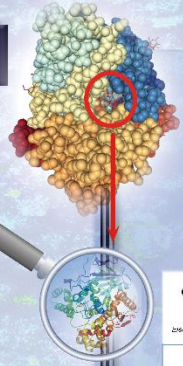
The primary **toxicity** of organophosphorus nerve agents results from the **inhibition** of the enzyme **Acetylcholinesterase (AChE)**.



AChE is responsible for breaking down the **neurotransmitter acetylcholine (ACh)**. This switches a nerve signal from on to off. If the enzyme is **inhibited**, ACh **accumulates** in the synapse and the signal **continues to transmit**.

Figure 1: Life Cycle of ACh.

Binding Site



The **AChE active site** is buried deep within the enzyme. It contains three amino acid residues **crucial for catalytic activity**: serine 200, histidine 440 and glutamate 327. The nerve agent binds to **serine 200**.

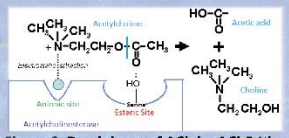


Figure 2: Breakdown of ACh by AChE (the normal function of the enzyme).

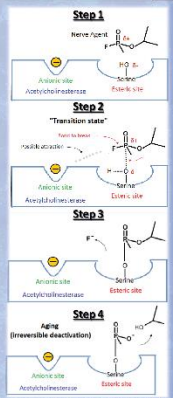
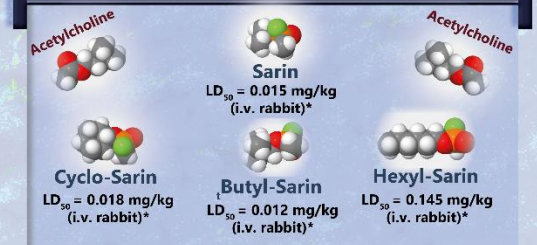
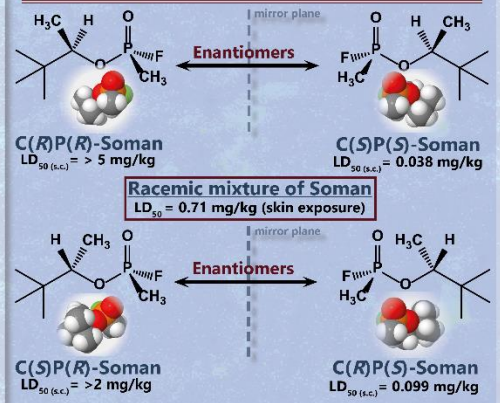


Figure 3: Mechanism of inhibition of AChE by Sarin.

Nerve Agent Molecular Shape and Size



Toxicity of an organophosphorus nerve agent depends on the ability to access the AChE binding site. **Size**, **shape** and **hydrophobicity** of the nerve agent exerts an effect. As alkyl substituents increase in size and degrees of freedom, toxicity decreases.



The **spatial orientation** (shape) of the molecule also matters, as illustrated by toxicity differences across the four stereoisomers of Soman.

Effects and Symptoms

Inhibition of AChE in muscarinic synapses (neuromuscular system) induces **cholinergic crisis**. Nicotinic synapses (central nervous system, e.g. brain) are also effected.

Symptoms include **sweating**, **salivation**, **miosis (pinpoint pupils)**, **paralysis**, **respiratory failure**, **seizures** and eventually **death**.

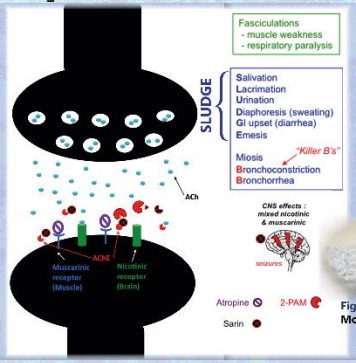
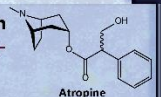


Figure 4: Inhibition of AChE by Sarin and Treatment with Atropine and 2-PAM.

Treatment

Atropine blocks the action of ACh at **muscarinic receptors** and treats **SLUDGE**.



Oximes such as **2-PAM** (pralidoxime) can reactivate inhibited AChE, but only before the aging process.
(Fig. 3, Step 3)

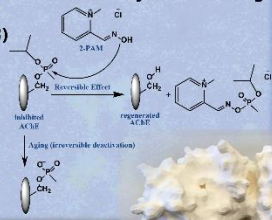


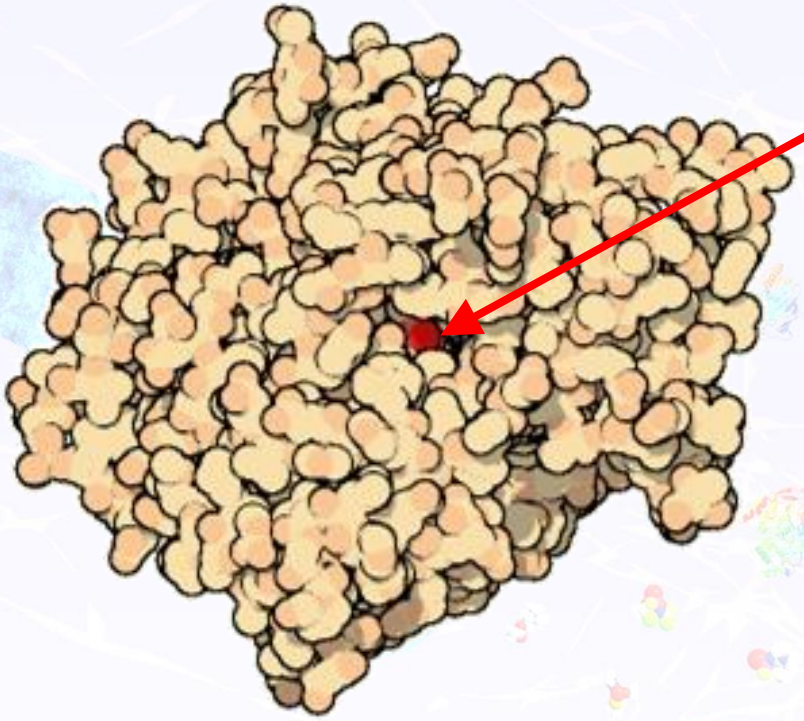
Figure 5: printed 3D Model of AChE

Figure 6: printed 3D Model of the AChE surface

Black, R. M., & Harrison, J. M. (2009). The Chemistry of Organophosphorus Chemical Warfare Agents. PATAI'S Chemistry of Functional Groups. doi:10.1002/9780470682531.pat0070

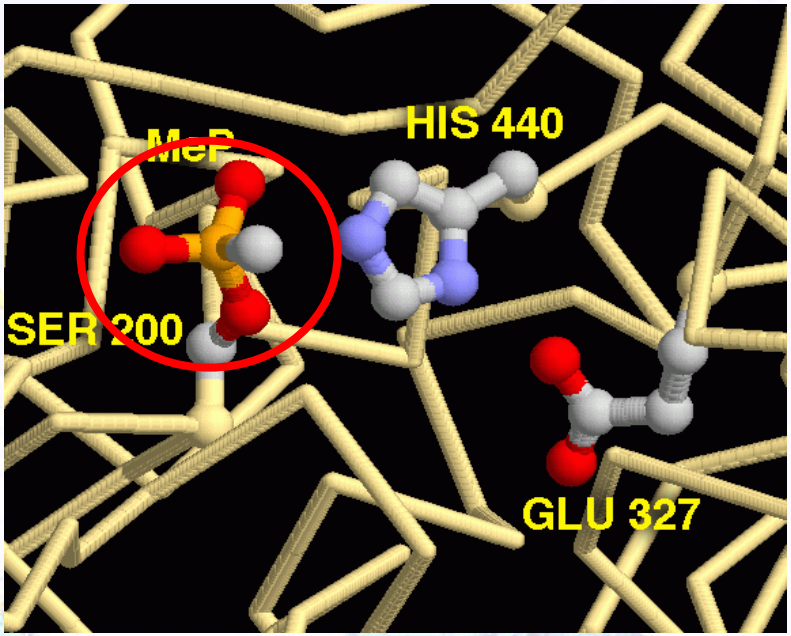
Broad Coverage Under a Schedule? What Does it Accomplish?

How Many 1A.01 Chemicals can Inhibit Acetylcholinesterase?



Binding pocket

Sarin adduct



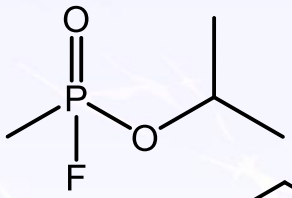
From PDB Molecule of the Month, 2004
https://pdb101.rcsb.org/motm/54

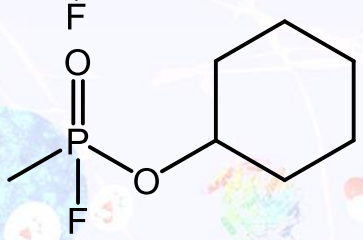
How Many 1A.01 Chemical can Inhibit Acetylcholinesterase?

C3/C1

Sarin

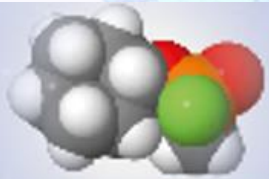
LD_{50} = 0.015 mg/kg
(i.v. rabbit)*





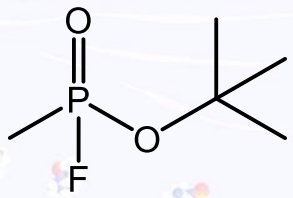
larger than sarin,
cyclo & branched alkyls
similar toxicity

C6/C1



Cyclo-Sarin

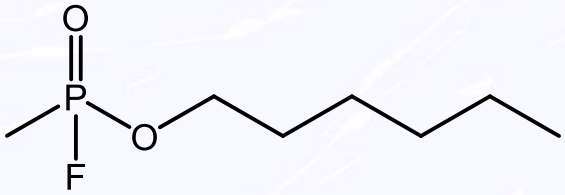
LD_{50} = 0.018 mg/kg
(i.v. rabbit)*



C4/C1

^{t}Butyl-Sarin

LD_{50} = 0.012 mg/kg
(i.v. rabbit)*



larger than sarin,
Linear alkyl group
lower toxicity

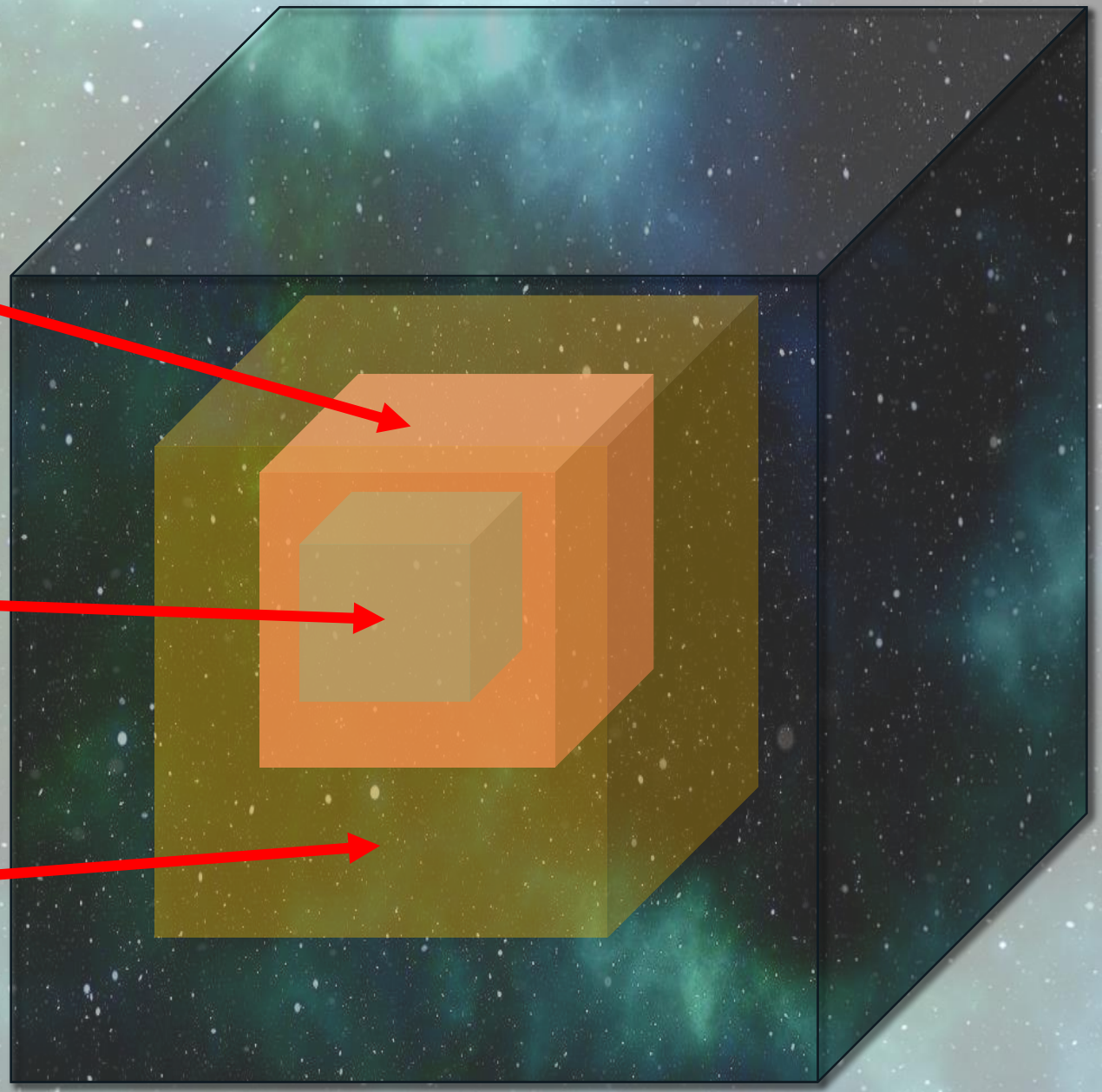
C6/C1

Hexyl-Sarin

LD_{50} = 0.145 mg/kg
(i.v. rabbit)*

Defining the Cn limit is all about capturing “Chemical Space”

All possible structures for R = H/C1 to C ∞



“Toxic Portion” (toxic family)

R ≤ Cn covers less space than “Toxic Portion” (smaller than toxic family)

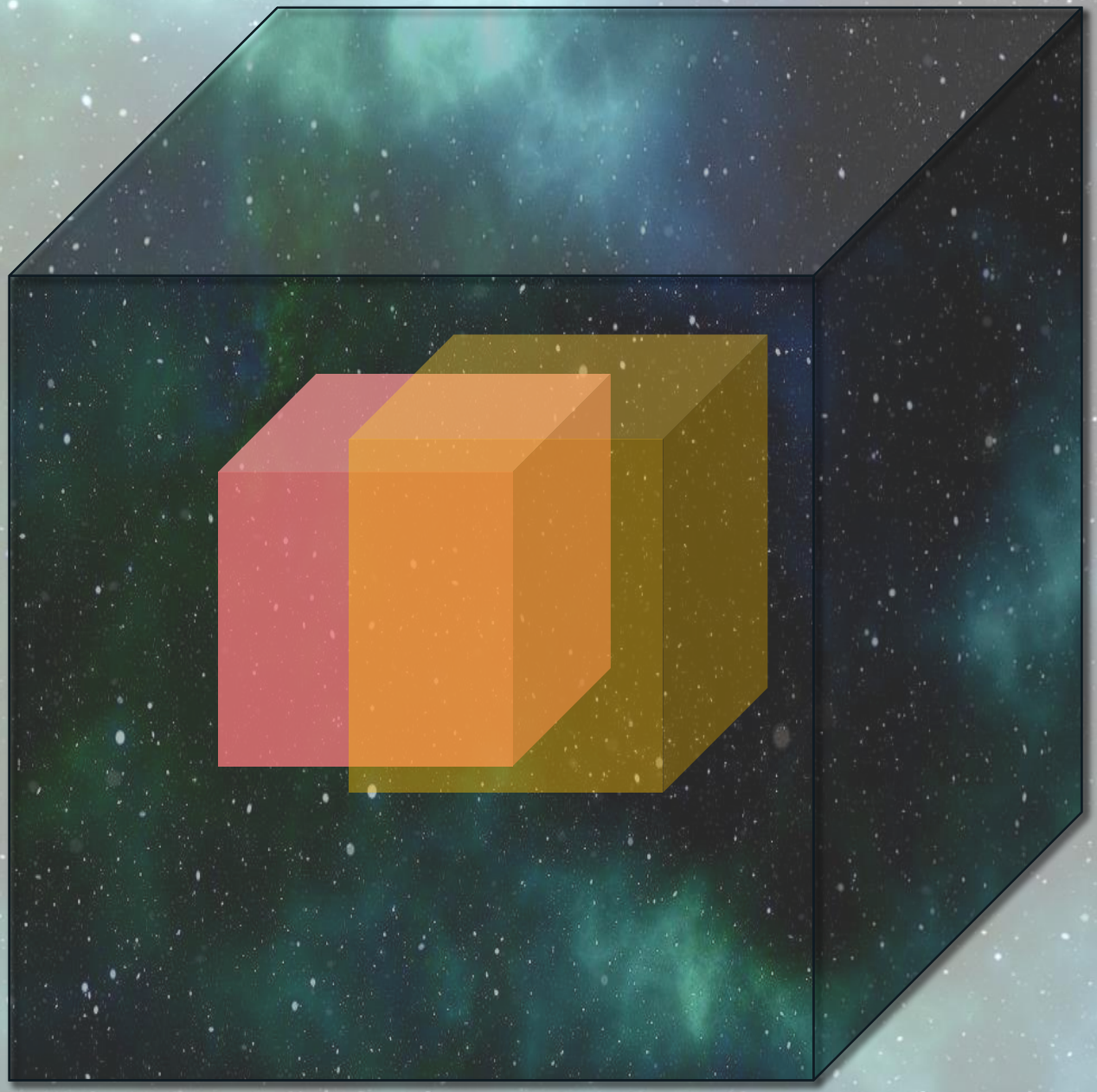
R ≤ Cn covers more space than “Toxic Portion” (larger than toxic family)

Can You Accurately Define Cn?

All possible structures for R = H/C1 to C ∞

"Toxic Portion" (toxic family)

R ≤ Cn overlaps but does not fully contain "Toxic Portion"



Do the Schedules Provide Guidance?

Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Schedule 1

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:

(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 is met:

(i) It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, toxic properties such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;

(ii) 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 1 Part A, Toxic Chemicals

1A(1) 1A(2) 1A(3) 1A(4) 1A(5) 1A(6) 1A(7) 1A(8)

Schedule 1 Part B, Precursors

1B(9) 1B(10) 1B(11) 1B(12)

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 1 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

2B(4) 2B(9) 2B(10) 2B(11) 2B(12) 2B(13) 2B(14)

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.

Schedule 3 Part A, Toxic Chemicals

3A(2) 3A(3) 3A(4) 3B(7) 3B(8) 3B(9) 3B(10) 3B(11) 3B(12) 3B(13) 3B(14) 3B(15) 3B(16) 3B(17)

Cast wide net – try to maximize the coverage of toxic chemical space (e.g. alkyls ≤ C10)

List individual toxic substances – yet there are many more possible biological toxins

Both approaches have their own merits and disadvantages

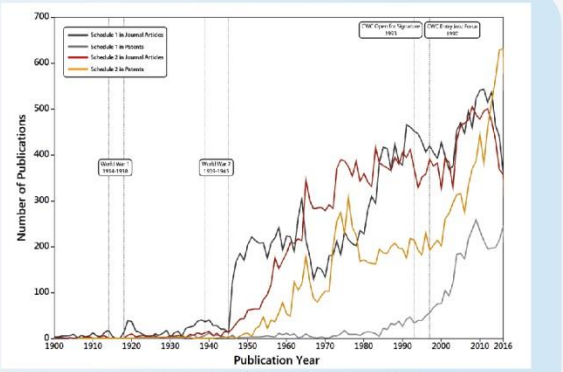
Schedule 3 (Used in production of Schedule 1 chemicals)

Schedule 2 (A Precursor) — Thiodiglycol 2B(13)

Thionyl chloride 3B(14)

Schedule 1 — Sulfur mustard 1A(4)

Relationship between Schedules, illustrated with sulfur mustard.



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.

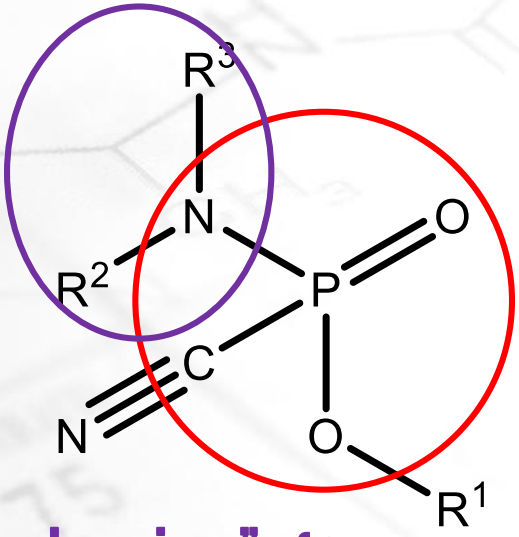
ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

@opcw @opcw_st /opcwonline /opcwonline /company/opcw /opcw

Other Families?

- **1A.02: *O*-Alkyl (≤ C10, incl. cycloalkyl) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidocyanidates**



"Dialkylamino" group (phosphoramido)

$R^1 \leq C_{10}$ alkyl, including cycloalkyl,
R^2, R^3 = Me, Et, n-Pr, i-Pr

"Phosphoro" not "Phosphono"

(no alkyl group connected to P atom)

	Me	Et	n-Pr	i-Pr
Me	Me Me	Me Et	Me n-Pr	Me i-Pr
Et	Et Me	Et Et	Et n-Pr	Et i-Pr
n-Pr	n-Pr Me	n-Pr Et	n-Pr n-Pr	n-Pr i-Pr
i-Pr	i-Pr Me	i-Pr Et	i-Pr n-Pr	i-Pr i-Pr

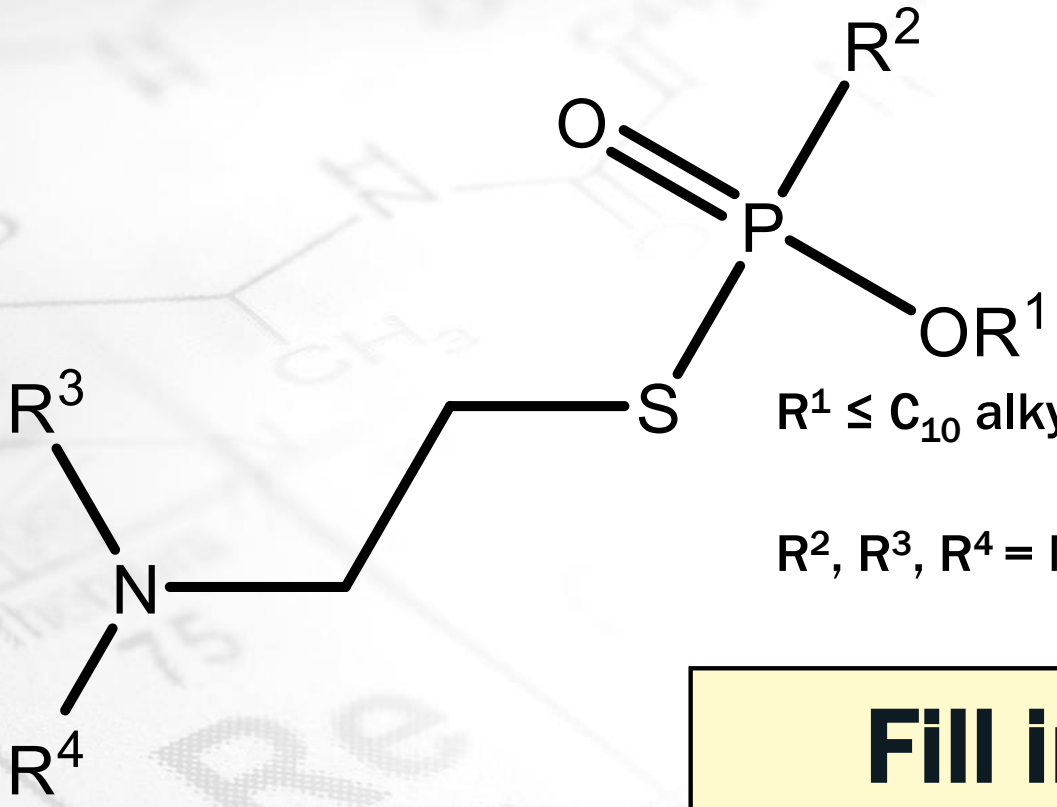
Duplicates of other asymmetric set

10 possibilities for dialkylamino group

10 (dialkylamino) X (> 1384 C1 to C10)

> 13,840 parent structures

Your Turn!



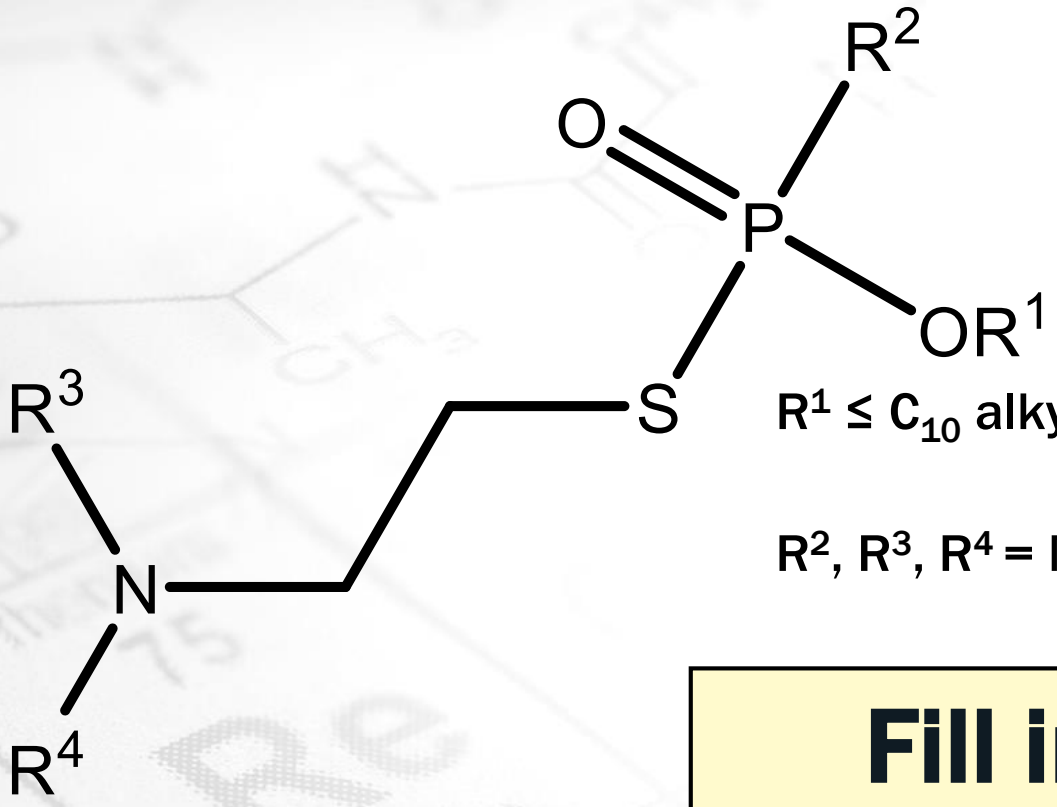
$R^1 \leq C_{10}$ alkyl, including cycloalkyl, alkyl

R^2, R^3, R^4 = Me, Et, n-Pr, i-Pr

Fill in the blank:

Phosphono Thiolate

Your Turn!



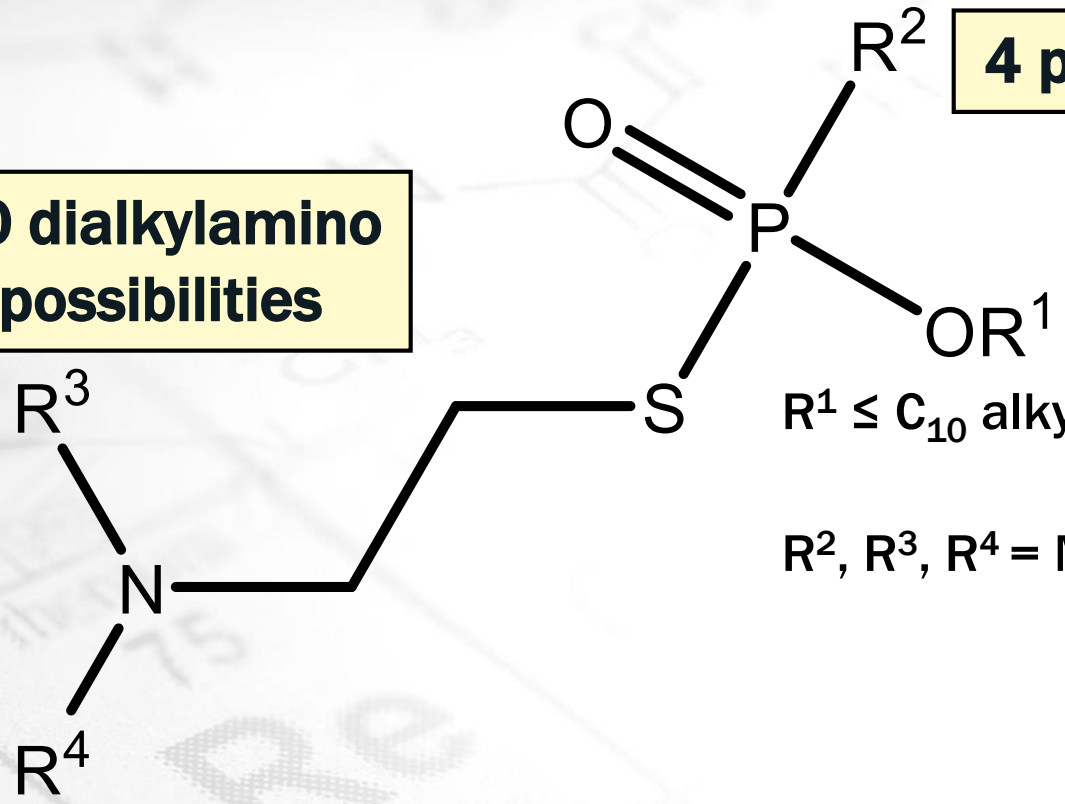
$R^1 \leq C_{10}$ alkyl, including cycloalkyl, alkyl

R^2, R^3, R^4 = Me, Et, n-Pr, i-Pr

Fill in the blank:

Phos_____ Thiolate

How Many Parent Structures?



4 possibilities

10 dialkylamino possibilities

> 1384 possibilities

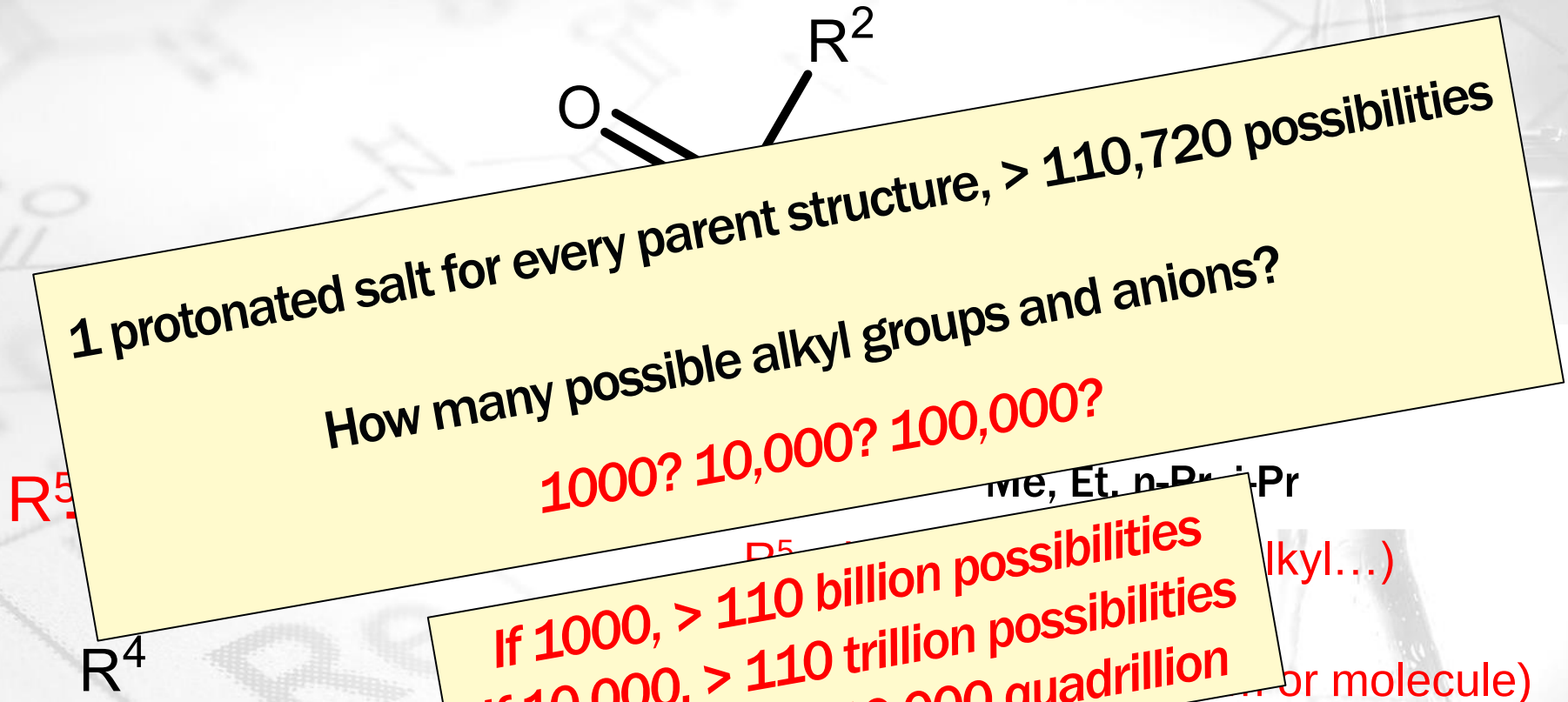
$R^1 \leq C_{10}$ alkyl, including cycloalkyl, alkyl

R^2, R^3, R^4 = Me, Et, n-Pr, i-Pr

10 (dialkylamino) X 4 X (> 1384 C1 to C10)

> 53,360 parent structures

And Just to Complicate Things, What Does Schedule 1A.03 Actually Say?



Me, Et, n-Pr, i-Pr

lkyl…)

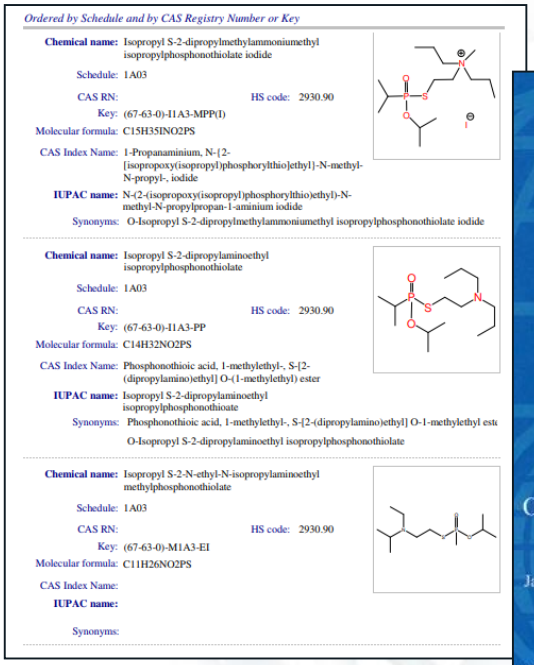
…or molecule)

***O*-Alkyl (H or s…, incl. cycloalkyl) S-2-dialkyl (Me, Et, n-Pr or i-Pr)-aminoethyl alkyl (Me, Et, n-Pr or i-Pr) phosphonothiolates and *corresponding alkylated or protonated salts*.**

How Many 1A.03 Chemicals Are Actually Known?

CAS®
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

- **CAS Database: 161 chemical substances**

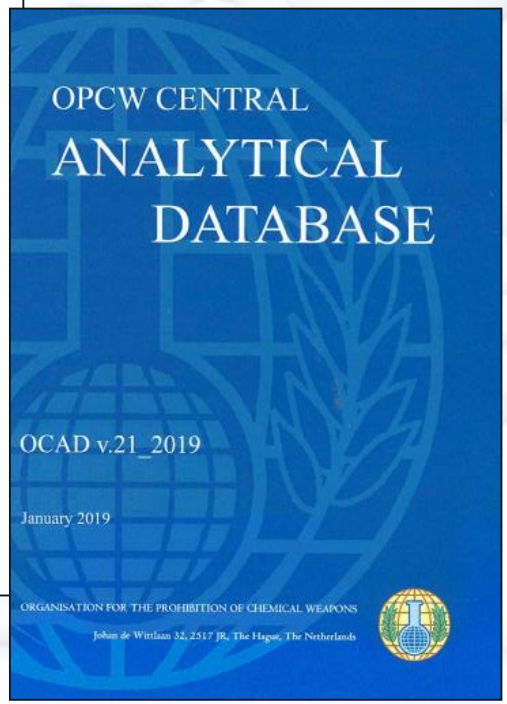


Ordered by Schedule and by CAS Registry Number or Key

Chemical name: Isopropyl S-2-dipropylmethylammoniumethyl isopropylphosphonothiolate iodide
Schedule: 1A03
CAS RN: HS code: 2930.90
Key: (67-63-0)-I1A3-MPP(I)
Molecular formula: C15H35INO2PS
CAS Index Name: 1-Propanaminium, N-[2-[isopropoxy(isopropyl)phosphorylthio]ethyl]-N-methyl-N-propyl-, iodide
IUPAC name: N-(2-(isopropoxy(isopropyl)phosphorylthio)ethyl)-N-methyl-N-propylpropan-1-aminium iodide
Synonyms: O-Isopropyl S-2-dipropylmethylammoniumethyl isopropylphosphonothiolate iodide

Chemical name: Isopropyl S-2-dipropylaminoethyl isopropylphosphonothiolate
Schedule: 1A03
CAS RN: HS code: 2930.90
Key: (67-63-0)-I1A3-PP
Molecular formula: C14H32NO2PS
CAS Index Name: Phosphonothioic acid, 1-methylethyl-, S-[2-(dipropylamino)ethyl] O-(1-methylethyl) ester
IUPAC name: Isopropyl S-2-dipropylaminoethyl isopropylphosphonothioate
Synonyms: Phosphonothioic acid, 1-methylethyl-, S-[2-(dipropylamino)ethyl] O-1-methylethyl este
O-Isopropyl S-2-dipropylaminoethyl isopropylphosphonothiolate

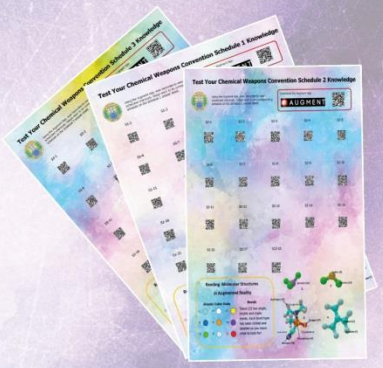
Chemical name: Isopropyl S-2-N-ethyl-N-isopropylaminoethyl methylphosphonothiolate
Schedule: 1A03
CAS RN: HS code: 2930.90
Key: (67-63-0)-M1A3-EI
Molecular formula: C11H26NO2PS
CAS Index Name:
IUPAC name:
Synonyms:



- **OPCW handbook on chemicals: 715 chemicals**

- **OCAD V21: 772 Mass Spectra**

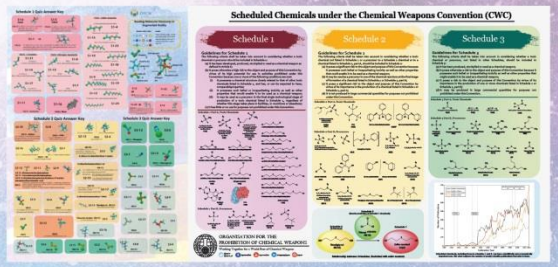
Take the Quiz!



Download the Quiz

Download the Answer Sheets

Download the Answer Key



Test your knowledge

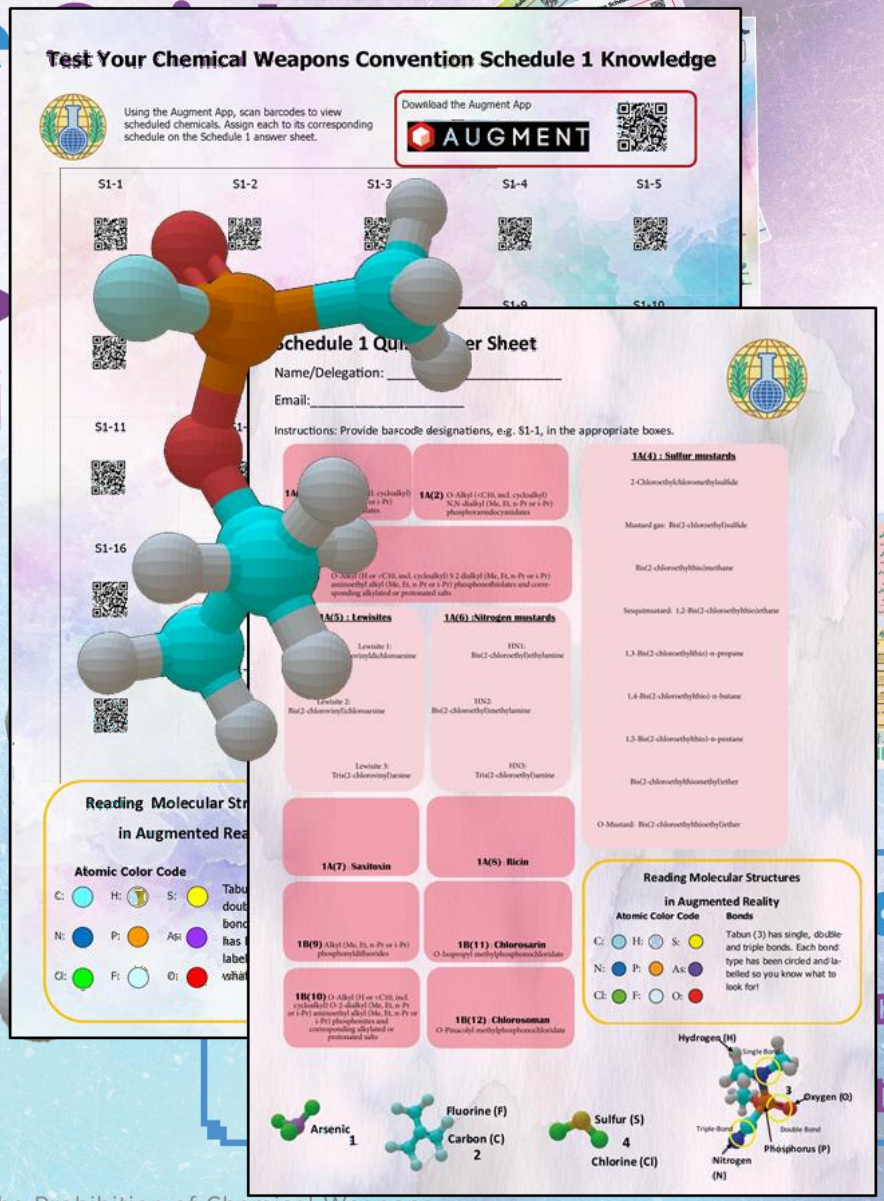
of the Schedules of the Chemical Weapons Convention

with an Augmented Reality Schedules quiz!

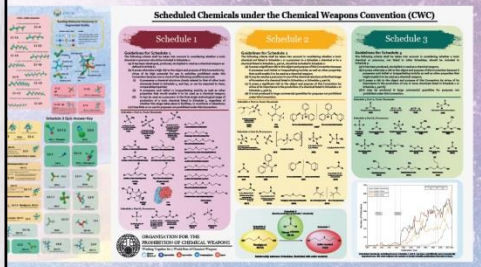
OPCW

Organisation for the Prohibition of Chemical Weapons

Take the



Download the Answer Sheets



owledge

cal Weapons Convention

ty Schedules quiz!

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Why Does All of This Matter?

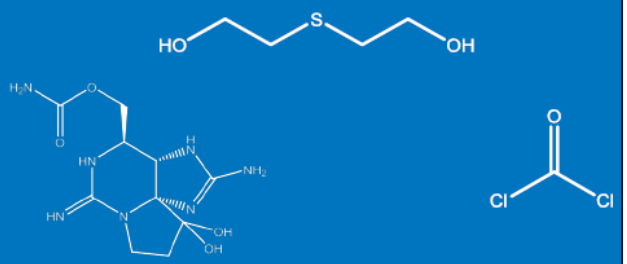
- **Technical issues require sound technical inputs**
- **All of the nuances required to understand what Schedules and their content represent in terms of chemistry came up in the recent Article XV discussions and evaluations**
- **Don't let the technical jargon be a hindrance!**
- ***Ice-cream and prizes***

Making Helpful Information More Accessible!

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

C. **SCHEDULES OF CHEMICALS**

The following Schedules list toxic chemicals and their precursors. I
implementing this Convention, these Schedules identify chemicals
of verification measures according to the provisions of the V
Pursuant to Article II, subparagraph 1 (a), these Schedules do not co
of chemical weapons.

Individual Schedules are defined by a general formula for a chem
specific chemical compounds. Associated chemical structures[2] and
Service (CAS) numbers are also included. Some of the chemicals
3D structure in "augmented reality" that can be viewed by scann
Augmented reality QR codes are identified by '(A)'.

Whenever reference is made to groups of dialkylated chemicals, fo
alkyl groups in parentheses, all chemicals possible by all possible co
groups listed in the parentheses are considered as listed in the resp
long as they are not explicitly exempted. A chemical marked "*" o
A, is subject to special thresholds for declaration and verification,
VII of the Verification Annex.

Scientific Advisory Board Recommendations

Chemical Abstract Service (CAS) numbers should not solely be rel
chemicals covered by the schedules. Although relevant as aids
verification, CAS numbers are not the only means to identify
determine whether a chemical is included in or excluded fr

[2] These have been added to provide additional information to the contents of the An
not part of the official Annex on Chemicals of the Chemical Weapons Convention.

[3] Viewing 3D molecular structures in augmented reality requires the use of the "An
is available for download to a mobile device from the "Play Store" (Android) or the

[4] See: *Response to the Direction-General's Request to the Scientific Advisory Boa
Advice on Scheduled Chemicals* (SAB-23/WP.1, dated 28 of April
www.opcw.org/sites/default/files/documents/SAB/en/sab-23-wp01_e_.pdf.

[5] For further information see: "Advice from the Scientific Advisory Board of th
Prohibition of Chemical Weapons on Isotopically Labelled Chemicals and Stereoisomers in Relation to
the Chemical Weapon Convention", C. M. Timperley, J. E. Forman, M. Abdollahi, A.S. Al-Amri, I. P.
Alonso, A. Baulig, V. Borrett, Veronica Borrett, F. A. Cariño, C. Curty, D. Gonzalez, Z. Kovarik, R.
Martinez-Alvarez, R. Mikulak, N. M. Fusaro Mouriño, P. Ramasami, S. Neffe, S. K. Raza, V. Rubaylo,
K. Takeuchi, C. Tang, F. Trifiro, F. Mauritz van Straten, P. S. Vanninen, V. Zaitsev, F. Waqar, M. Said
Zina, S. Holen, H. A. Weinstein; *Pure Appl. Chem.*, 2018, *90(10)*, 1647-1670. DOI: 10.1515/pac-2018-
0803.

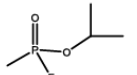
Schedule 1 (CAS registry number)

A. Toxic chemicals:

(1) ***O*-Alkyl (≤ C_{10}, incl. cycloalkyl) alkyl (Me, Et, n-Pr or i-Pr)-phosphonofluoridates**

$R^1 \leq C_{10}$, including cycloalkyl, alkyl
R^2 = Me, Et, n-Pr, i-Pr

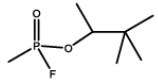
e.g. Sarin: *O*-Isopropyl methylphosphonofluoridate (107-44-8)



R^1 = i-Pr
R^2 = Me

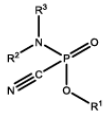
(A)

Soman: *O*-Pinacolyl methylphosphonofluoridate (96-64-0)



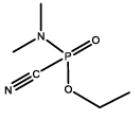
R^1 = Pinacolyl (3,3-dimethyl-2-butyl)
R^2 = Me

(2) ***O*-Alkyl (≤ C_{10}, incl. cycloalkyl) *N,N*-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidocyanidates**



$R^1 \leq C_{10}$, including cycloalkyl, alkyl
R^2, R^3 = Me, Et, n-Pr, i-Pr

e.g. Tabun: *O*-Ethyl *N,N*-dimethyl phosphoramidocyanidate (77-81-6)



R^1 = Et
R^2, R^3 = Me

(A)

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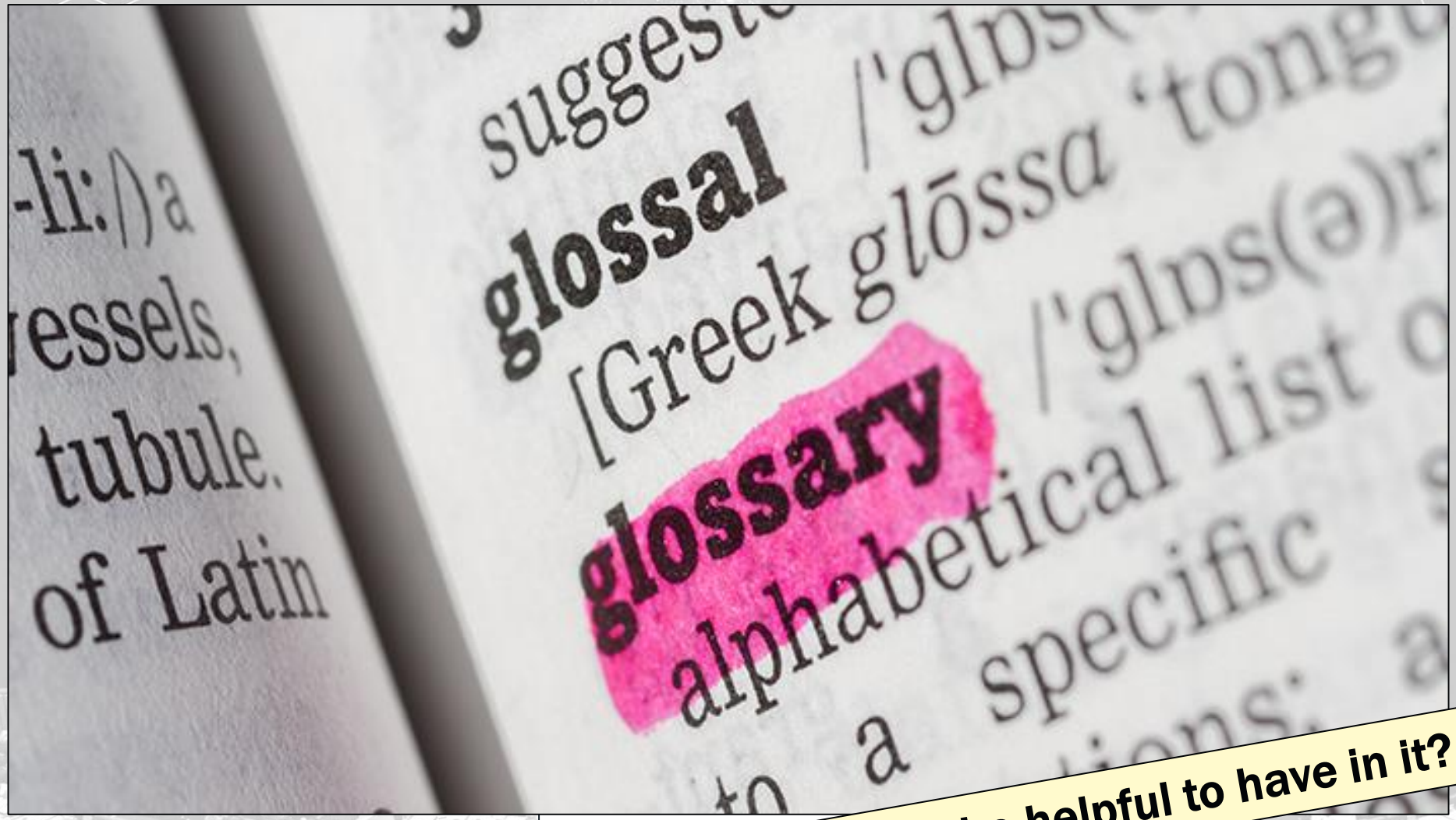
Making Helpful Information More Accessible!



What would be helpful to have in it?

Answers from Particpants

Where do We Go from Here?

Where do We Go from Here?


New Chair and Vice-Chair for 2019

- SAB will meet from 11 – 14 June
- TWG will meet in April, September (TBC) and November (TBC)

Look for Continued Technical Secretariat Engagement in 2019 as Well!

Science for Diplomats at EC-89

Suitability for Fieldwork: The Science and Technology of Physical Protection

Are you as agile as an OPCW Inspector?
Join us to find out!

Tuesday 9 October
13:30 – 14:45
Ooms Room
Light lunch available at 13:00

Science Advice, Science Diplomacy and Science Communication at the Organisation for the Prohibition of Chemical Weapons

Scientific Advisory Board

The Chemical Weapons Convention is built on a scientific foundation, requiring technical expertise for effective implementation, and scientific literacy for decision making.

Scientific principles provide the definitions for what is, and what is not a chemical weapon; ensure completeness of declarations; guarantee the robustness of sampling and analysis and other verification methodologies; guide the processes and methods used for inspections, investigations and destruction; inform approaches to assistance and protection; and benefits outreach to scientific communities."

The Scientific Advisory Board (SAB) is a subsidiary body of the OPCW serving as an independent science advisory mechanism to provide advice to inform the work and processes of the OPCW, and to bring scientific literacy into the policymaking process.

The SAB was established in accordance with the Chemical Weapons Convention to enable the Director-General to render specialized advice in areas of science and technology relevant to the Convention, its State Parties, the Conference of States Parties, and the Executive Council.

For the basis of the SAB in the Chemical Weapons Convention, see Article VIII Paragraph 21 (h).

Scientific Diplomacy in Support of the Convention

Nationalities of Members of the SAB and its Working Groups 1998 - 2018

The SAB is made up of 25 experts from OPCW Member States. Members serve in their personal capacity (not as representatives of their respective States Parties) for up to two consecutive three-year terms. The SAB chair and vice-chair are elected annually.

Scientists from more than 40 States Parties have served on the SAB and/or its working groups since its first Session in 1998. Upholding the core values of the Convention, international cooperation and science for peace, the SAB exemplifies the value of science diplomacy.

OPCW Designated Laboratory network in April 2018

International scientific collaboration to support the implementation of the Chemical Weapons Convention is further exemplified by the network of Designated Laboratories.

Learn more about Designated Labs

Work of the SAB from January to July 2018

The SAB reports to the Director-General, who provides responses and views on its work and recommendations. States Parties receive the reports and the responses through the Director-General.

Find out more

Reports of SAB | Other

SAB

Science Communication and Engagement

OPCW actively promotes scientific literacy for policymaking and treaty implementation. This requires productive discourse between scientific experts and diplomats from OPCW's State Parties.

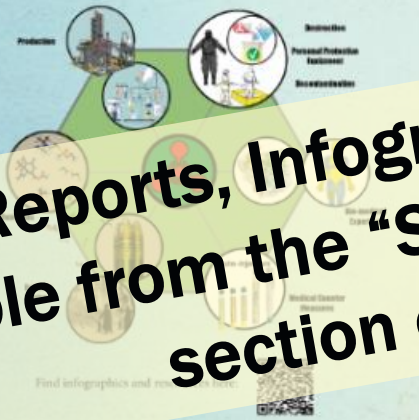
The SAB regularly briefs States Parties on its work and the OPCW's Science for Diplomats initiative provides a forum for interactive engagement with diplomats involved in the implementation of the Chemical Weapons Convention.

Learn more about the "Science for Diplomats Initiative"

To ensure effectiveness, the work of the SAB must be visible; SAB reports and informative materials must be easily accessible to stakeholders; and the promotion of scientific literacy must be interactive and engaging.

Mobile apps, mobile device retrievable documents and augmented reality provide useful tools with a great degree of flexibility to aid in communication and dissemination of information.

Science of the Chemical Weapons Convention



Scientific Review for the Fourth Review Conference of the Chemical Weapons Convention

The Scientific Advisory Board serves as an independent body that assesses and reports to the Director-General on developments in scientific and technological fields relevant to the Convention. Recognising where technological change both benefits and challenges the implementation of the Convention is an important and continual aspect of this work (in particular for verification purposes).

To ensure the OPCW keeps pace with scientific and technological change, the SAB submits a substantive report on developments in science and technology which includes recommendations for the operation of the Convention to each 5-yearly Review Conference of the Chemical Weapons Convention. The upcoming Fourth Review Conference (RC-4) is to be held from 21 – 30 November 2018.

The SAB took inputs for its report to RC-4 from previous considerations to the first three Review Conferences, engagement within scientific conferences and meetings, review of scientific and patent literature, and a variety of new sources that included **A-D** below.

Read the Executive Summary of Recommendations to RC-4

RC4 report
RC-4/DG.1
30 April 2018

A. The deliberations of the SAB during its eight regular sessions held from June 2013 to March 2018 (SAB-20 to SAB-27)

- Report of the Scientific Advisory Board at its 27th Session (SAB-27/1, dated 23 March 2018)
- Director-General's Response to the Report of the 27th Session of the Scientific Advisory Board (EC-86/DG.5, dated 9 May 2018)
- Report of the Scientific Advisory Board at its 26th Session (SAB-26/1, dated 20 October 2017)
- Director-General's Response to the Report of the 26th Session of the Scientific Advisory Board (EC-87/DG.11, dated 23 January 2018)
- Report of the Scientific Advisory Board at its 25th Session (SAB-25/1, dated 31 March 2017)
- Director-General's Response to the Report of the 25th Session of the Scientific Advisory Board (EC-83/DG.8, dated 19 May 2017)
- Report of the Scientific Advisory Board at its 24th Session (SAB-24/1, dated 28 October 2016)
- Director-General's Response to the Report of the 24th Session of the Scientific Advisory Board (EC-84/DG.9, dated 18 January 2017)
- Report of the Scientific Advisory Board at its 23rd Session
- Report of the Scientific Advisory Board at its 22nd Session
- Director-General's Response to the Report of the 21st Session of the Scientific Advisory Board (EC-77/DG.10, dated 5 September 2014)
- Report of the Scientific Advisory Board at its 20th Session (SAB-20/1, dated 14 June 2013)
- Director-General's Response to the Report of the 20th Session of the Scientific Advisory Board (EC-78/DG.1, dated 24 July 2013)

B. Findings from four Temporary Working Groups

DG response
RC-4/DG.2
1 June 2018

C. Intersessional responses to requests for advice from the Director-General (2013 to 2017)

Medical countermeasures and longer term treatment for victims of chemical agent exposure

Toxicologically labeled and stereoisomers of Scheduled chemicals

Simple storage and

D. A series of workshops, co-organised by external partners and kindly funded by the European Union

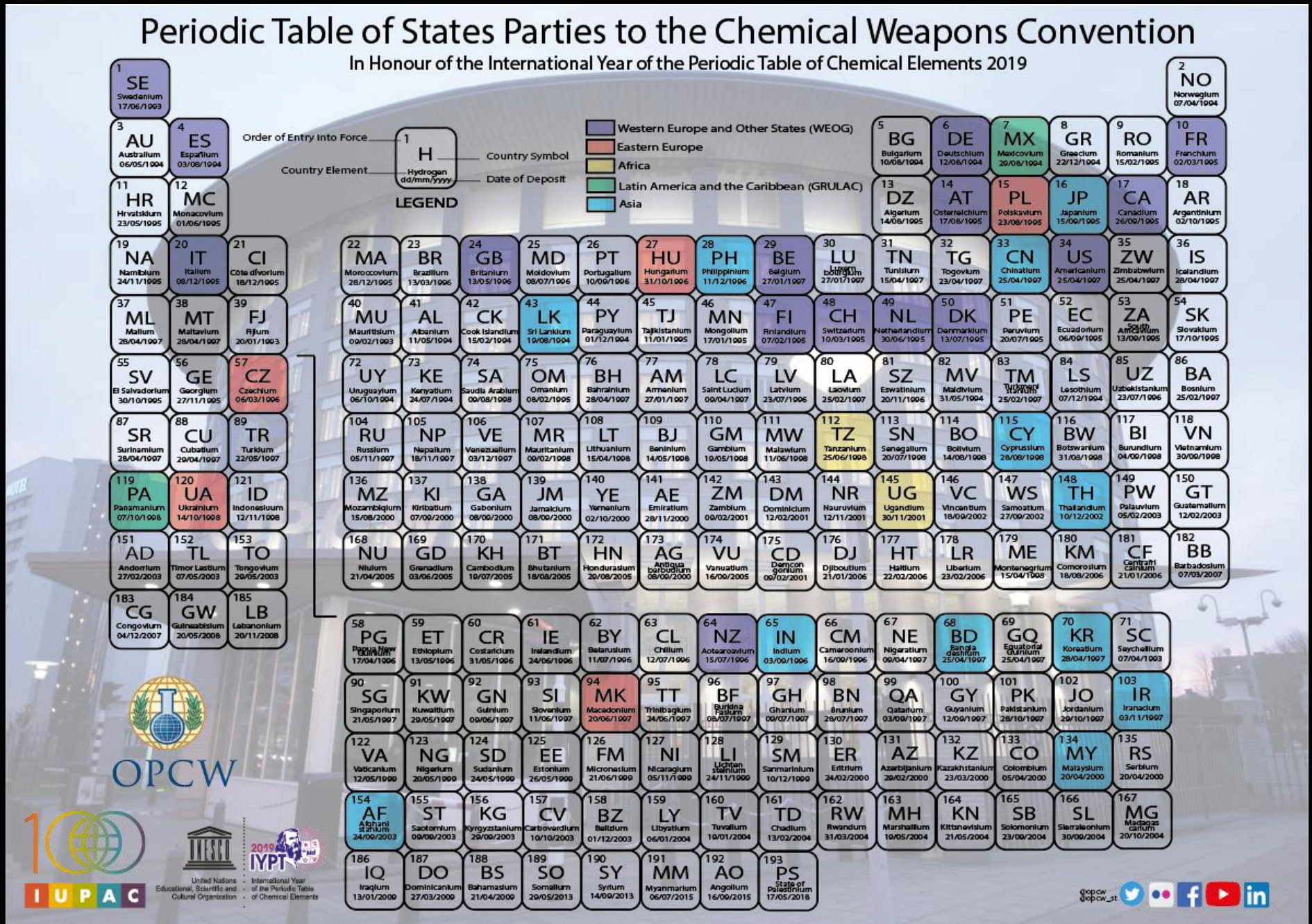
Examples of the topics covered in the report include the convergence the sciences, chemical production and technology to enhance capability.

Download these graphics and explore with augmented reality!

Reports, Infographics and More Available from the "Science and Technology" section of OPCW.org

OPCW
Organisation for the Prohibition of Chemical Weapons

Thank You for Joining In!




ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

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