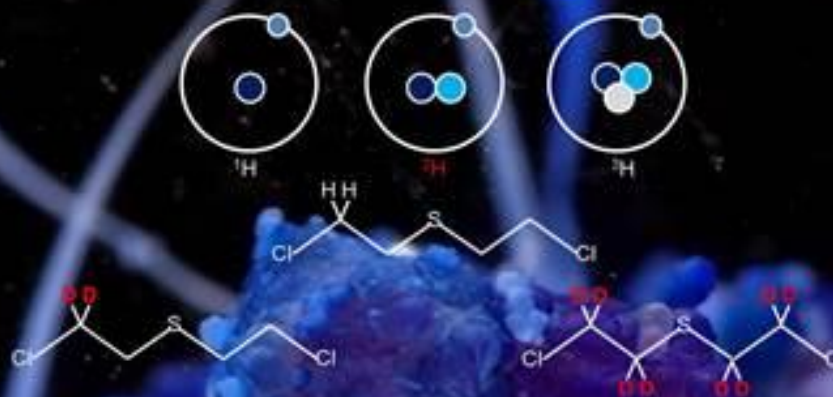


SCIENCE FOR DIPLOMATS

ISOTOPIC LABELS, STEREOISOMERS, & SCHEDULED CHEMICALS

WHY DOES THIS MATTER? A REVIEW OF THE SAB'S ADVICE

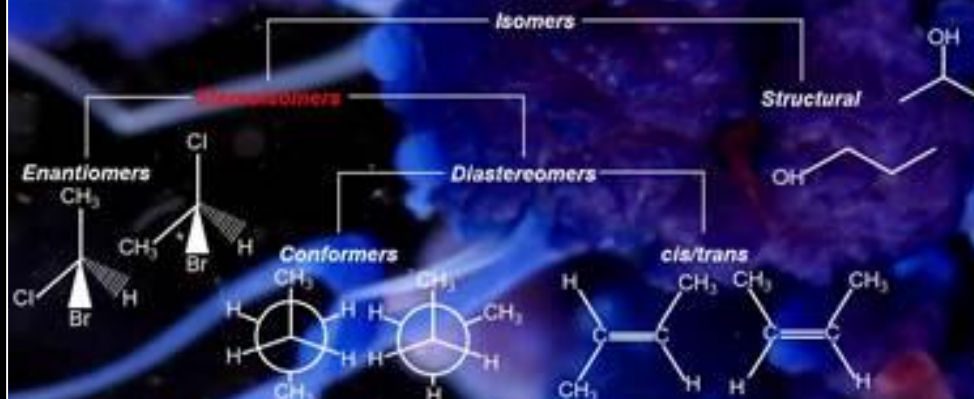


WEDNESDAY 13 JULY 2016

13:30-15:00

OOMS ROOM

LIGHT LUNCH PROVIDED AT 13:00





At SAB-22, The Director-General requested the Scientific Advisory Board (SAB) to:

- make technical recommendations on **isotopic labelling** of chemicals relevant to Schedule 1, 2 and 3 under the Chemical Weapons Convention – in light of the SAB's previous advice on CAS registry numbers (RC-2/DG.1, dated 28 February 2008, in paragraph 3.5 of the Annex);
- assess whether the chemical properties of a chemical are altered, when subject to isotopic labelling, in a manner that would affect its relevance to the schedules of chemicals under the Chemical Weapons Convention; and
- make technical recommendations on how **stereoisomers** of chemicals relevant to Schedule 1, 2 and 3 under the Chemical Weapons Convention should be considered in relation to the Convention, taking into account the SAB's previous advice on CAS registry numbers (RC-2/DG.1, dated 28 February 2008, in paragraph 3.5 of the Annex).



At SAB-22, The Director-General requested the Scientific Advisory Board (SAB) to:

- make technical recommendations on **isotopic labelling** of chemicals relevant to S... light of
the... ed 28
Feb...
- asse... , when
subj... e to the
sche...
- mak... relevant
to S... ould be
considered in relation to the Convention, taking into account the SAB's
previous advice on CAS registry numbers (RC-2/DG.1, dated 28 February
2008, in paragraph 3.5 of the Annex).



OPCW

Scientific Advisory Board

Twenty - Third Session
18 – 22 April 2016

SAB-23/WP.1
28 April 2016
ENGLISH only

**RESPONSE TO THE DIRECTOR-GENERAL'S REQUEST TO THE
SCIENTIFIC ADVISORY BOARD TO PROVIDE FURTHER ADVICE
ON SCHEDULED CHEMICALS**



**RESPONSE TO THE DIRECTOR-GENERAL'S REQUEST TO THE
SCIENTIFIC ADVISORY BOARD TO PROVIDE FURTHER ADVICE
ON SCHEDULED CHEMICALS**

1. RECOMMENDATIONS

- 1.1 The Scientific Advisory Board (SAB) has considered isotopically labelled scheduled chemicals and stereoisomers of scheduled compounds relating to the Convention according to the Director-General's requests (see Appendixes 1 and 2).
- 1.2 **Recommendation 1.** The SAB recommends that the molecular parent structure of a chemical should determine whether it is covered by a schedule entry. This is because:
- (a) it is inappropriate to rely solely upon Chemical Abstracts Service (CAS) numbers to define chemicals covered by the schedules. Although relevant as aids to declaration and verification, CAS numbers should not be used as the means to identify a chemical, or to determine whether a chemical is included in, or excluded from, a schedule;
 - (b) thus, if a chemical is included within a schedule, then all possible isotopically-labelled forms and stereoisomers of that chemical should be included, irrespective of whether or not they have been assigned a CAS number or have CAS numbers different to those shown in the Annex on Chemicals to the Convention. The isotopically labelled compound or stereoisomer related to the parent chemical specified in the schedule should be interpreted as belonging to the same schedule; and
 - (c) this advice is consistent with previous SAB views on this topic.¹
- 1.3 **Recommendation 2.** Inclusion of appropriate analytical data in the Central Agent Database (OCAD) for isotopically labelled relatives of scheduled chemicals where available is recommended.

¹

RG-2/DG.1, dated 28 February 2008, in paragraph 3.5 of its Annex.





Part 1: Chemical Abstracts Service (CAS) Registry Number?

Is a unique numeric identifier

Designates only one substance

Contains no chemical information, yet is a link to a wealth of information about a specific chemical substance

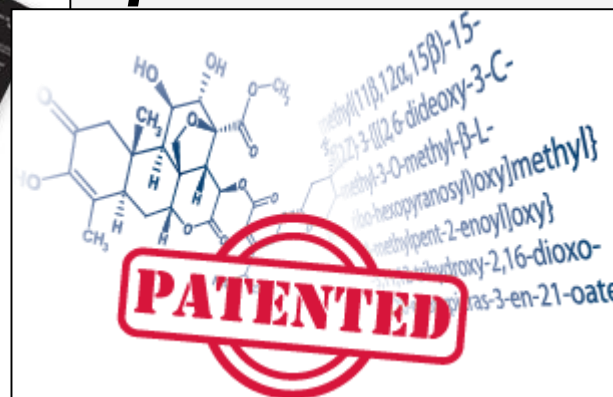


Part 1: Chemical Abstracts Service (CAS) Registry Number?

Is a
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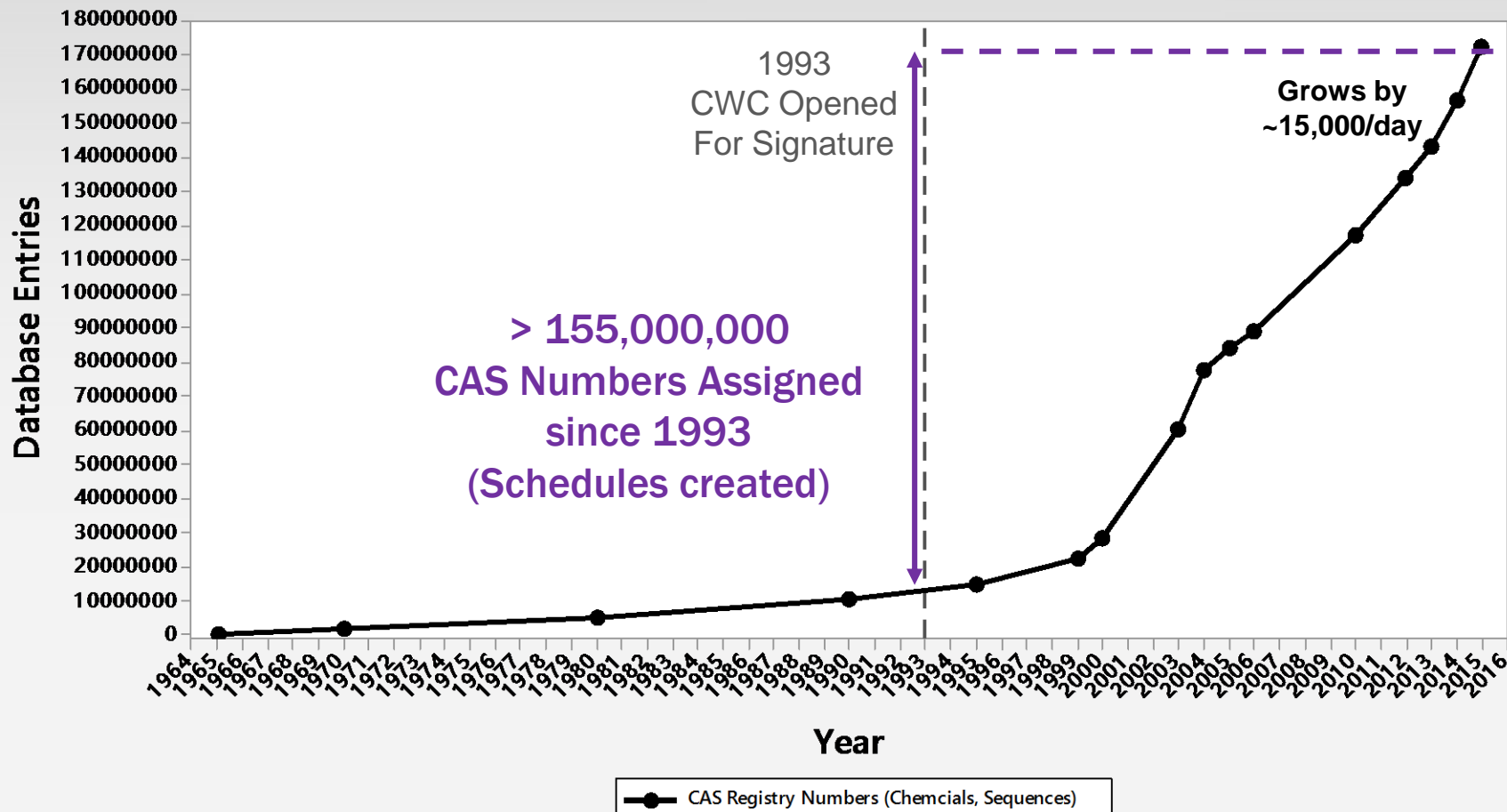


on, yet is a link to
specific





How Many CAS Registry Numbers Have Been Assigned?



Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Schedule 1

Guidelines for Schedule 1

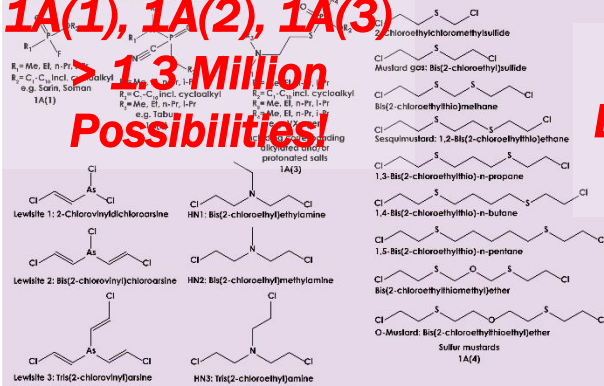
The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:

- It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:
 - It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparable properties;
 - It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;
 - 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;
- It has little or no use for purposes not prohibited under this Convention.

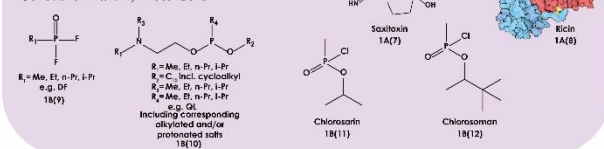
Schedule 1 Part A, Toxic Chemicals

1A(1), 1A(2), 1A(3)

> 1.3 Million Possibilities!



Schedule 1 Part B, Precursors



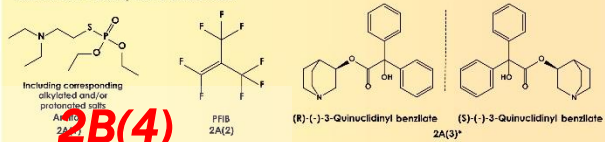
Schedule 2

Guidelines for Schedule 2

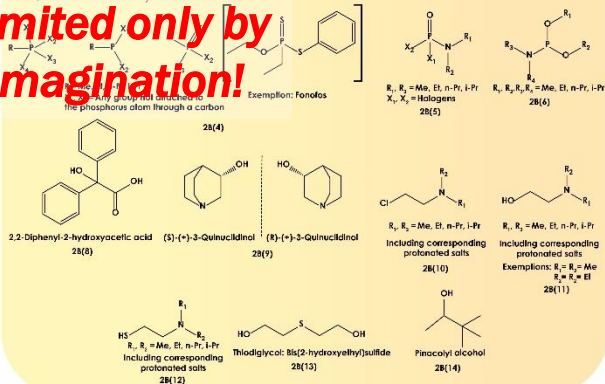
The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:

- 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;
- 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;
- 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;
- It is not produced in large commercial quantities for purposes not prohibited under this Convention.

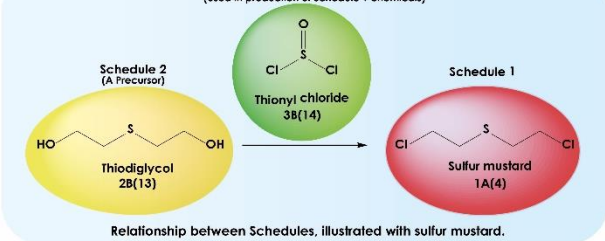
Schedule 2 Part A, Toxic Chemicals



Schedule 2 Part B, Precursors



Schedule 3 (Used in production of Schedule 1 chemicals)



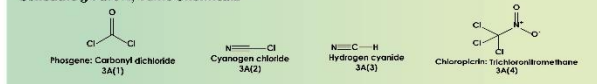
Schedule 3

Guidelines for Schedule 3

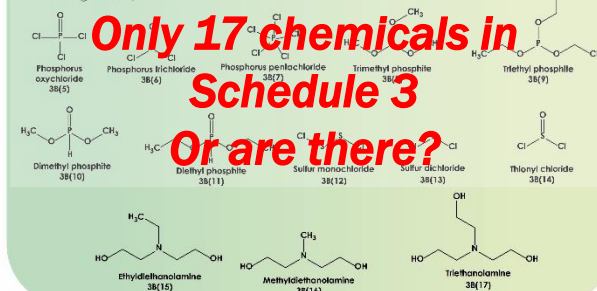
The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

- It has been produced, stockpiled or used as a chemical weapon;
- 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;
- 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;
- It may be produced in large commercial quantities for purposes not prohibited under this Convention.

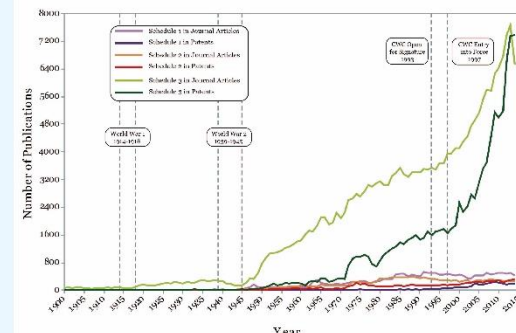
Schedule 3 Part A, Toxic Chemicals



Schedule 3 Part B, Precursors



Only 17 chemicals in Schedule 3 Or are there?



Scheduled chemicals are both scientifically and economically important as illustrated by the number of yearly publications that refer to them.

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

Scheduled Chemicals under the Chemical Weapons Convention (CWC)

Schedule 1

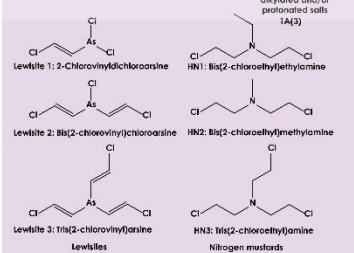
Guidelines for Schedule 1

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

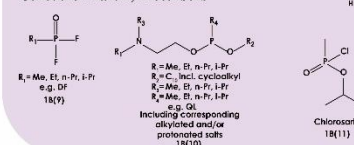
- It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;
- It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:
 - It possesses a chemical structure of chemicals listed in Schedule 1, and comparable properties;
 - It possesses such lethal or incapacitating properties that would enable it to be used as a chemical weapon;
 - It may be used as a precursor in the production of a toxic chemical listed in Schedule 1, whether this stage takes place in fact or not;
- It has little or no use for purposes not prohibited by this Convention.

Schedule 1 Part A, Toxic Chemicals

1A(1), 1A(2), 1A(3), 1A(4), 1A(5)
> 1.3 Million Possibilities!



Schedule 1 Part B, Precursors

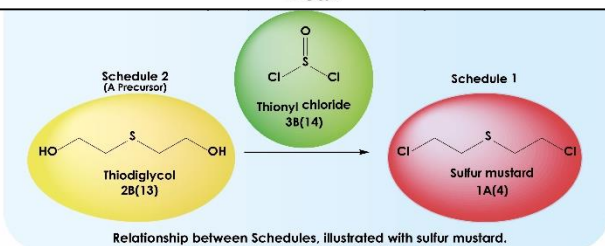
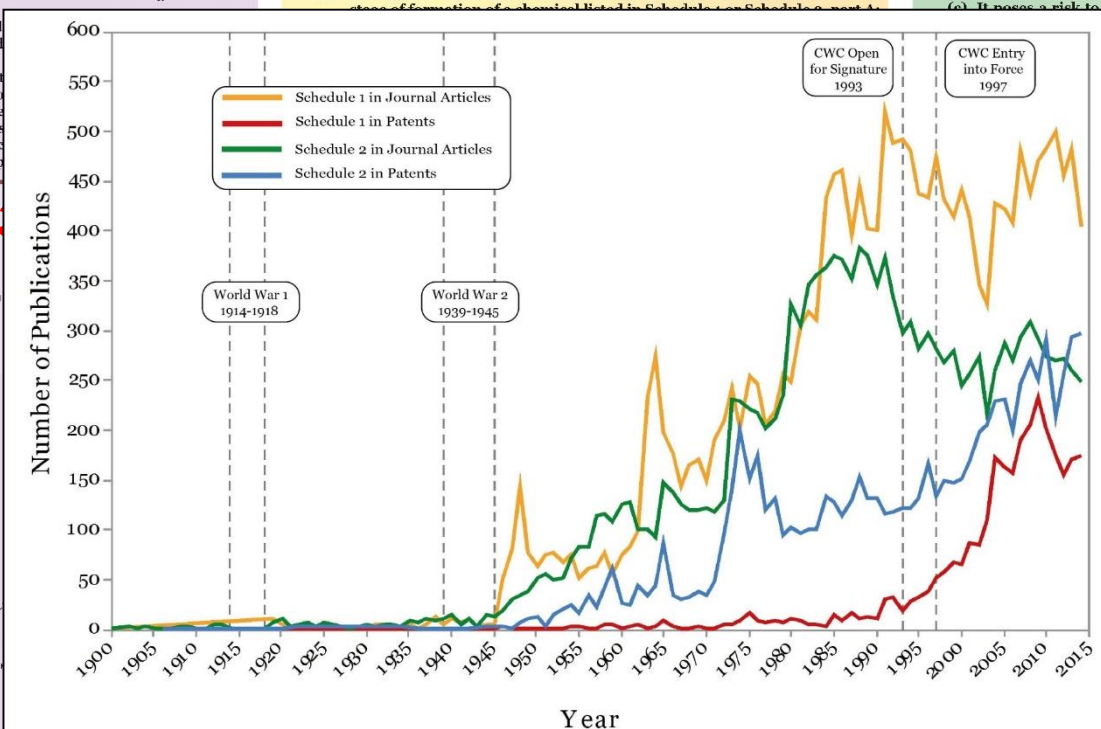


Schedule 2

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 a chemical listed in Schedule 2, part A, should be included in Schedule 2:

- 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;
- 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 a chemical listed in Schedule 2, part A.

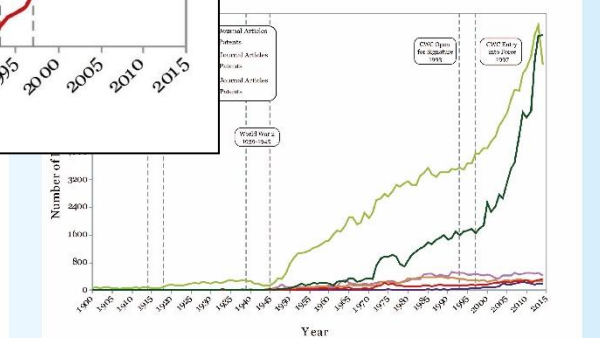
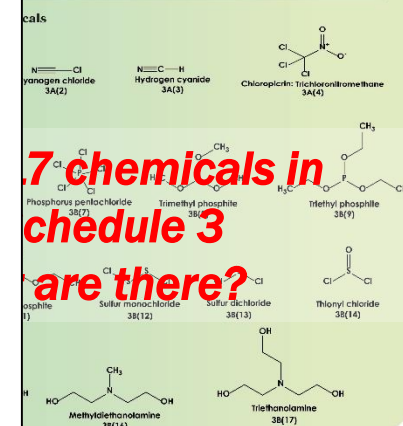


Schedule 3

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:

- It has been produced, stockpiled or used as a chemical weapon;
- 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;
- It poses a risk to the object and purpose of this Convention by virtue of the production of one or more chemicals listed in Schedule 2, part B; or
- It is produced in large commercial quantities for purposes not prohibited by this Convention.



Scheduled chemicals are both scientifically and economically important as illustrated by the number of yearly publications that refer to them.

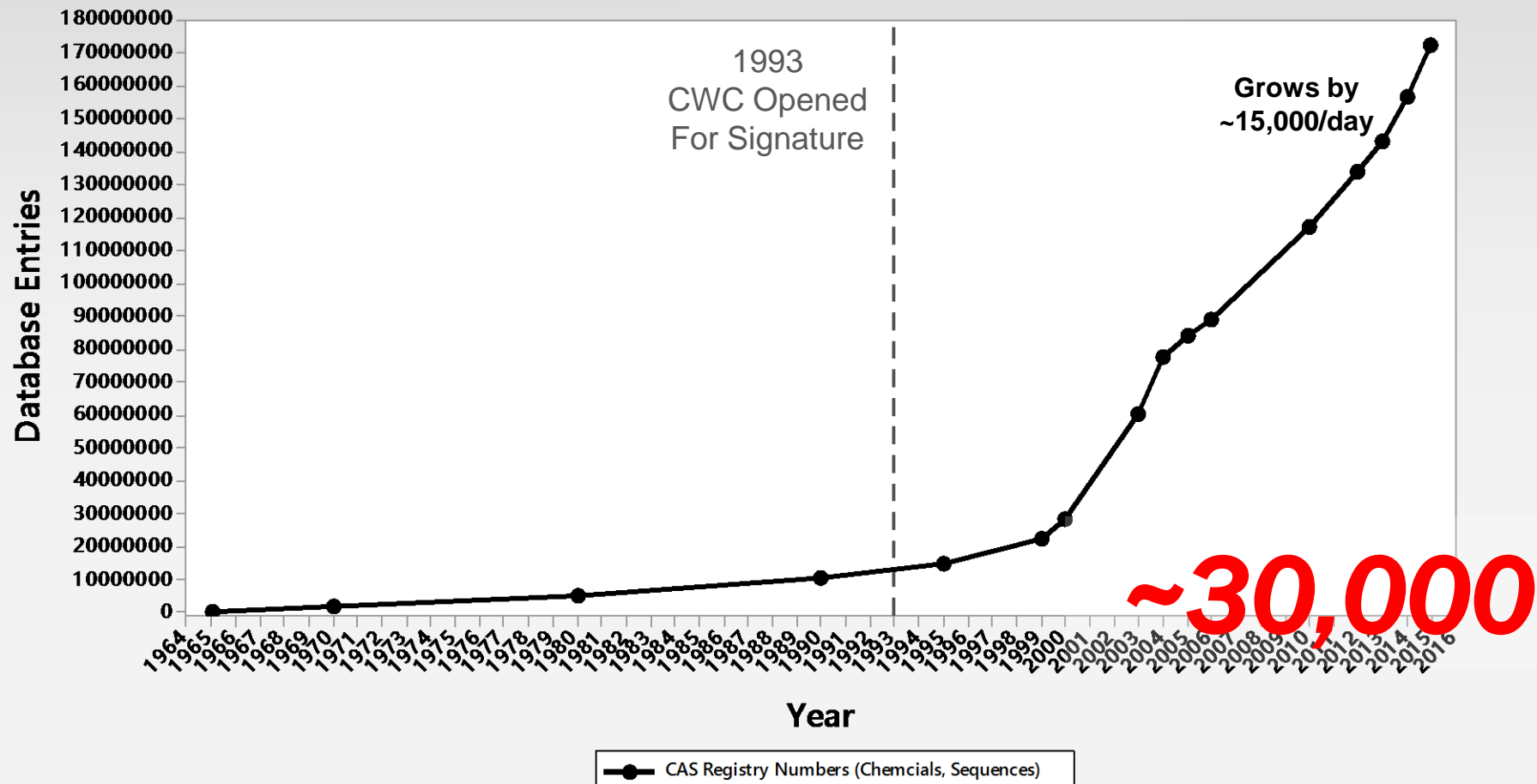


ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working Together for a World Free of Chemical Weapons

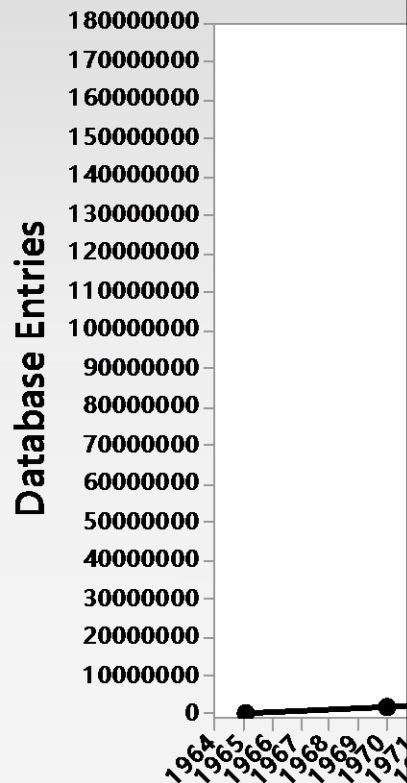


How Many Scheduled Chemicals Have CAS Registry Numbers?





How Many Scheduled Chemicals Have CAS Registry Numbers?



Schedule 1

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 (91-44-6)

- (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)

(CAS registry
number)

**55 in Annex
on Chemicals
(3 are not
Scheduled)**

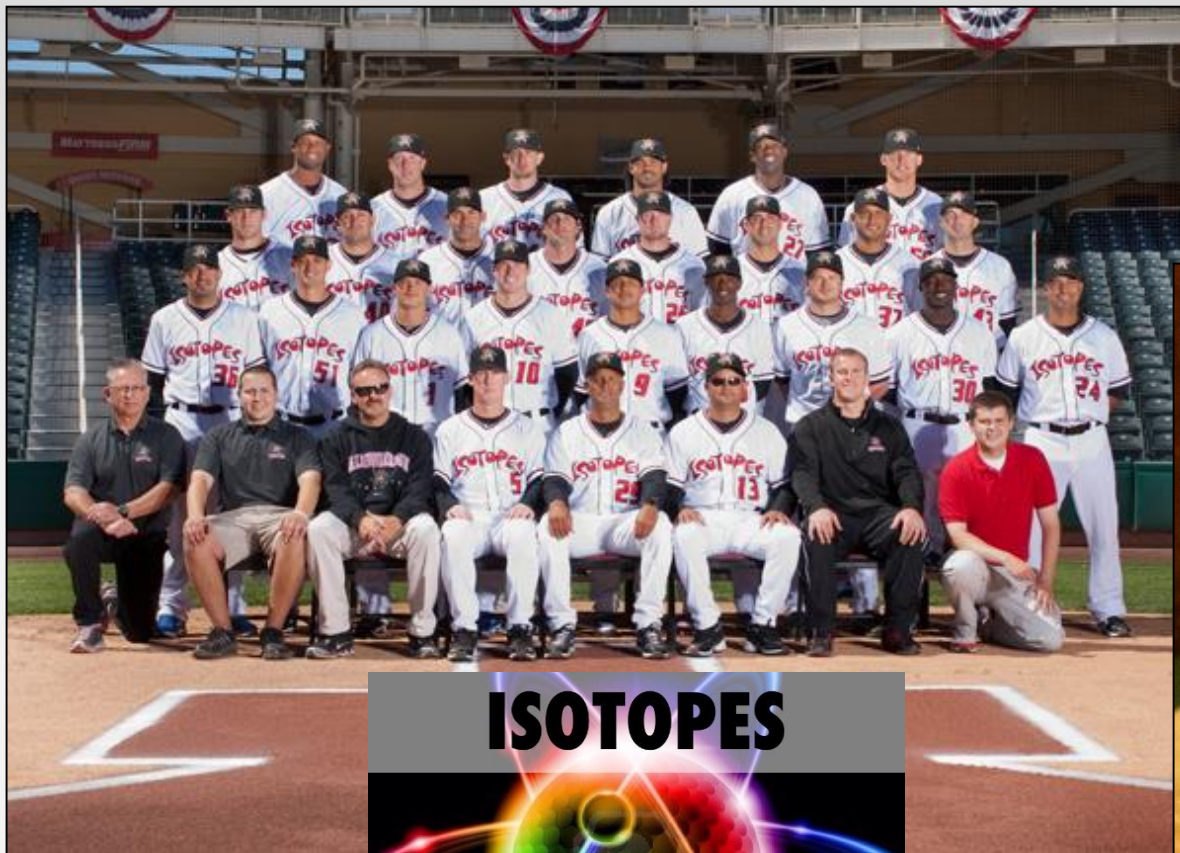
Grows by
~15,000/day

30,000

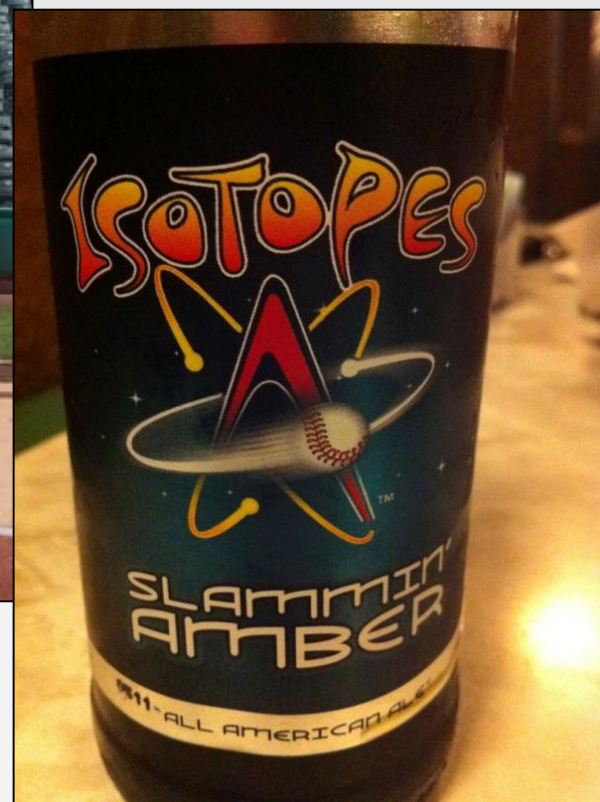
2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016



Part 2: Isotopes

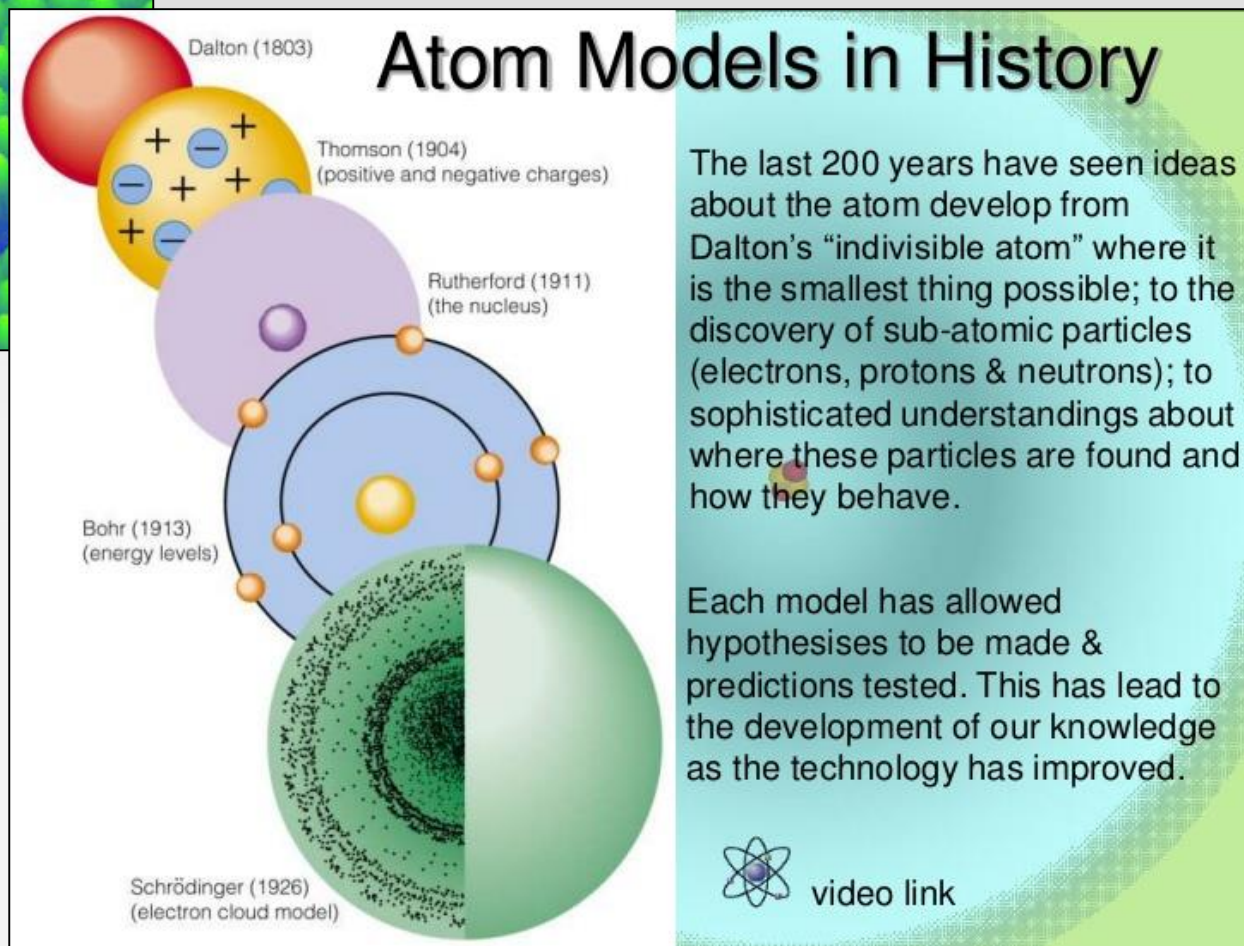
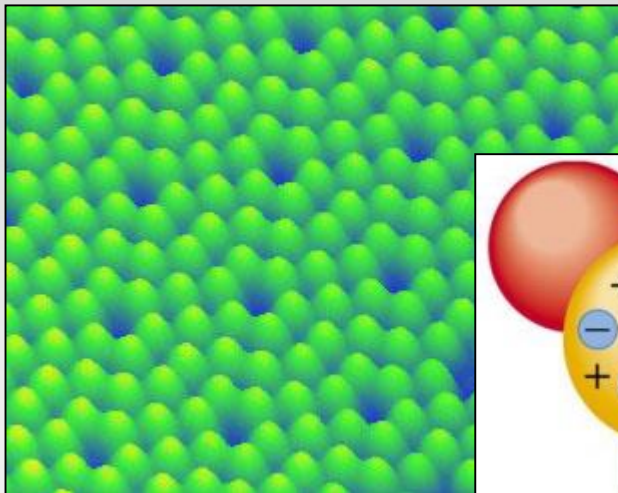


ISOTOPES





But First Atoms...

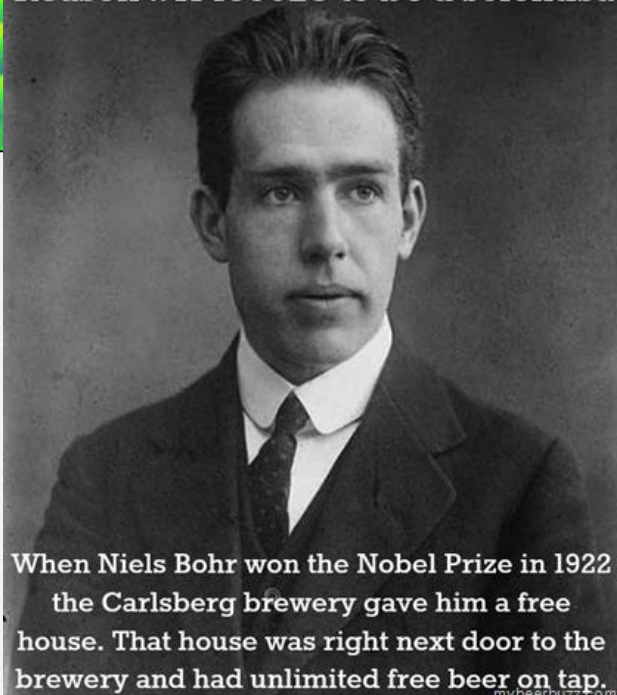




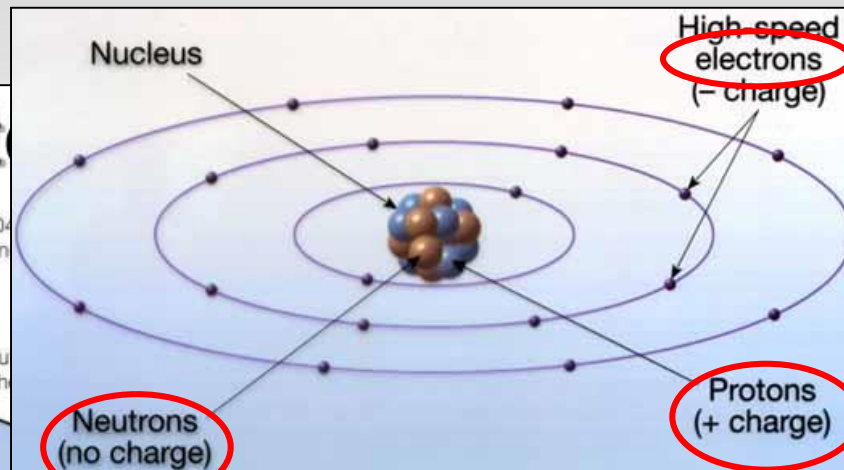
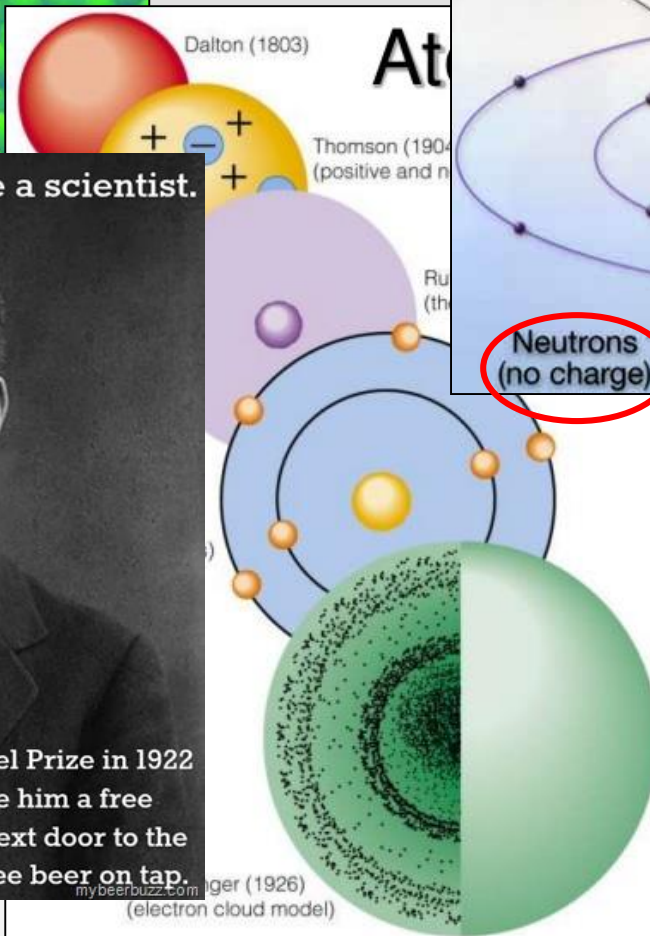
But First Atoms...



Reason #17483028 to be a scientist.



When Niels Bohr won the Nobel Prize in 1922 the Carlsberg brewery gave him a free house. That house was right next door to the brewery and had unlimited free beer on tap.



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

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



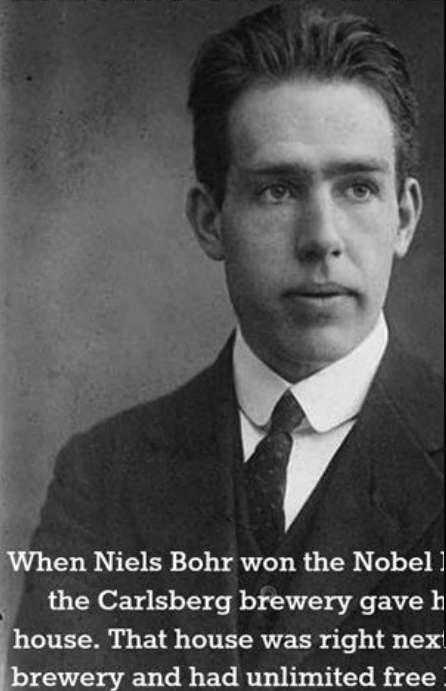
video link



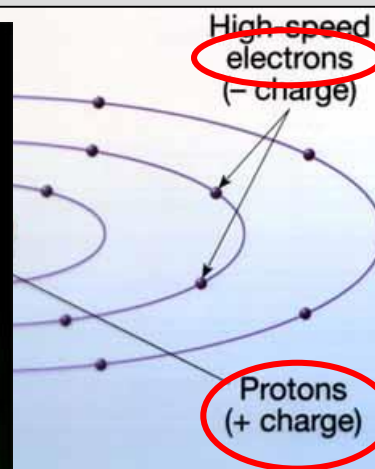
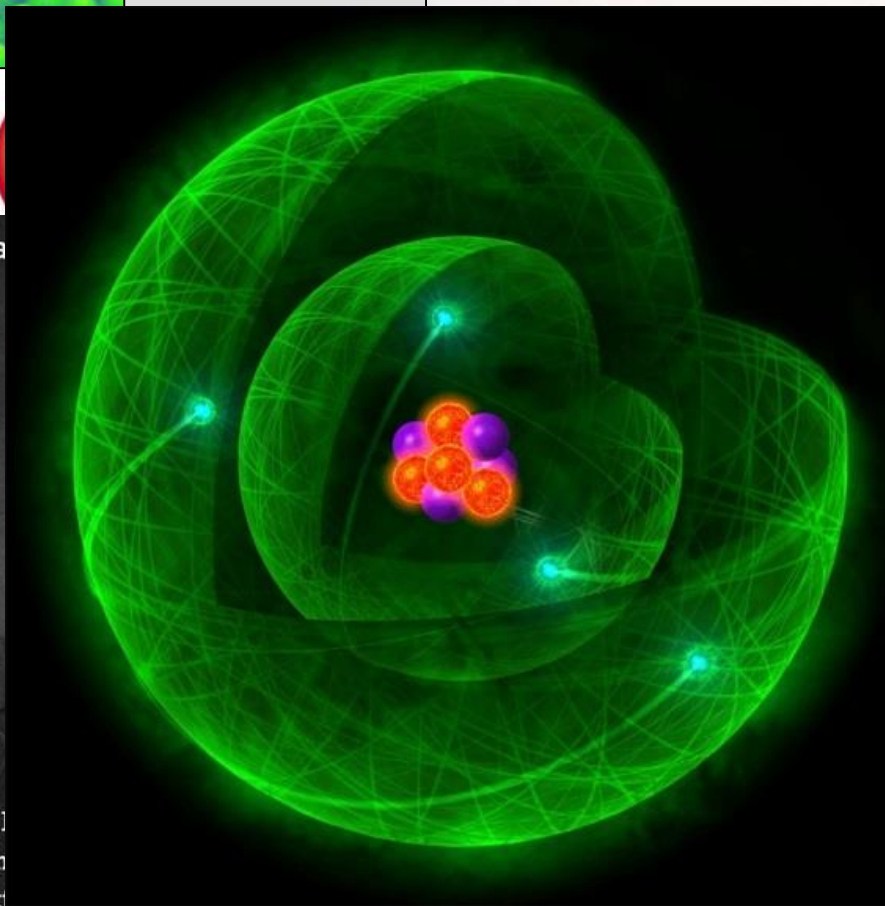
But First Atoms...



Reason #17483028 to be a



When Niels Bohr won the Nobel Prize in 1922, the Carlsberg brewery gave him a house. That house was right next to the Carlsberg brewery and had unlimited free beer on tap.



Understandings about particles are found and improved.

As allowed to be made & used. This has led to a great deal of our knowledge and technology has improved.



video link



And Elements...

IUPAC Periodic Table of the Elements

1

①

H

hydrogen

[1.007, 1.009]

2

Key:

atomic number

Symbol

name

standard atomic weight

13

14

15

16

17

18

3

Li

lithium

[6.938, 6.997]

4

Be

beryllium

9.012

11

Na

sodium

22.99

12

Mg

magnesium

[24.30, 24.31]

19

K

potassium

39.10

20

Ca

calcium

40.08

21

Sc

scandium

44.96

22

Ti

titanium

47.87

23

V

vanadium

50.94

24

Cr

chromium

52.00

25

Mn

manganese

54.94

26

Fe

iron

55.85

27

Co

cobalt

58.93

28

Ni

nickel

58.69

29

Cu

copper

63.55

30

Zn

zinc

[65.38(2)]

31

Ga

gallium

69.72

32

Ge

germanium

72.63

33

As

arsenic

74.92

34

Se

selenium

78.97

35

Br

bromine

[79.90, 79.91]

36

Kr

krypton

83.80

37

Rb

rubidium

85.47

38

Sr

strontium

87.62

39

Y

yttrium

88.91

40

Zr

zirconium

91.22

41

Nb

niobium

92.91

42

Mo

molybdenum

95.95

43

Tc

technetium

44

Ru

ruthenium

101.1

45

Rh

rhodium

102.9

46

Pd

palladium

106.4

47

Ag

silver

107.9

48

Cd

cadmium

112.4

49

In

indium

114.8

50

Sn

tin

118.7

51

Sb

antimony

121.8

52

Te

tellurium

127.6

53

I

iodine

126.9

54

Xe

xenon

131.3

55

Cs

caesium

132.9

56

Ba

barium

137.3

57-71

lanthanoids

72

Hf

hafnium

178.5

73

Ta

tantalum

180.9

74

W

tungsten

183.8

75

Re

rhenium

186.2

76

Os

osmium

190.2

77

Ir

iridium

192.2

78

Pt

platinum

195.1

79

Au

gold

197.0

80

Hg

mercury

200.6

81

Tl

thallium

[204.3, 204.4]

82

Pb

lead

207.2

83

Bi

bismuth

208.0

84

Po

polonium

85

At

astatine

86

Rn

radon

87

Fr

francium

88

Ra

radium

89-103

actinoids

104

Rf

rutherfordium

105

Db

dubnium

106

Sg

seaborgium

107

Bh

bohrium

108

Hs

hassium

109

Mt

meitnerium

110

Ds

darmstadtium

111

Rg

roentgenium

112

Cn

copernicium

113

Uut

ununtrium

114

Fl

flerovium

115

Uup

ununpentium

116

Lv

livermorium

117

Uus

ununseptium

118

Uuo

ununoctium

1 = Atomic Number = Number of Protons

Protons = Electrons (neutral atom)

57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.0	71 Lu lutetium 175.0
89 Ac actinium	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

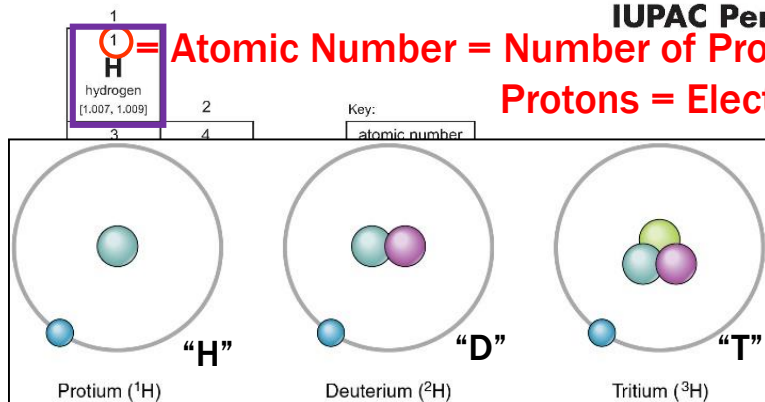


And Elements...

IUPAC Periodic Table of the Elements

Atomic Number = Number of Protons

Protons = Electrons (neutral atom)

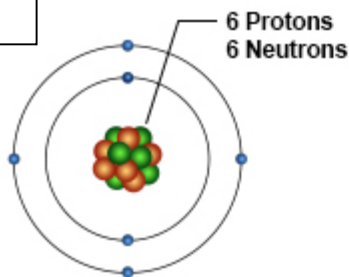


13	14	15	16	17	18
5 B boron [10.80, 10.83]	6 C carbon [12.00, 12.02]	7 N nitrogen [14.00, 14.01]	8 O oxygen [15.99, 16.00]	9 F fluorine 19.00	10 Ne neon 20.18
13	14	15	16	17	18

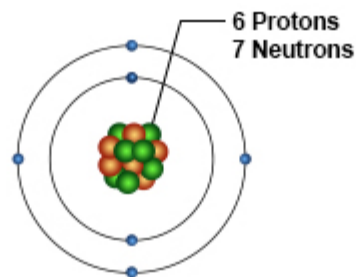
37 Rb rubidium 85.47	38 Sr strontium 87.62	39 Y yttrium 88.91	40 Zr zirconium 91.22	41 Nb niobium 92.91	42 Mo molybdenum 95.95	43 Tc technetium
55 Cs caesium 132.9	56 Ba barium 137.3	57-71 lanthanoids	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.8	75 Re rhenium 186.2
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium

57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2
89 Ac actinium	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0

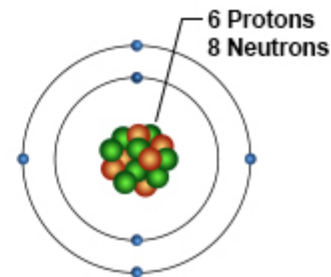
NATURAL ISOTOPES OF CARBON



Carbon-12
(6P + 6N)
Atomic Weight = 12
Isotope Mass: 12 u
Abundance: 98.89%



Carbon-13
(6P + 7N)
Atomic Weight = 13
Atomic Mass = 13.00335 u
Abundance: 1.109%

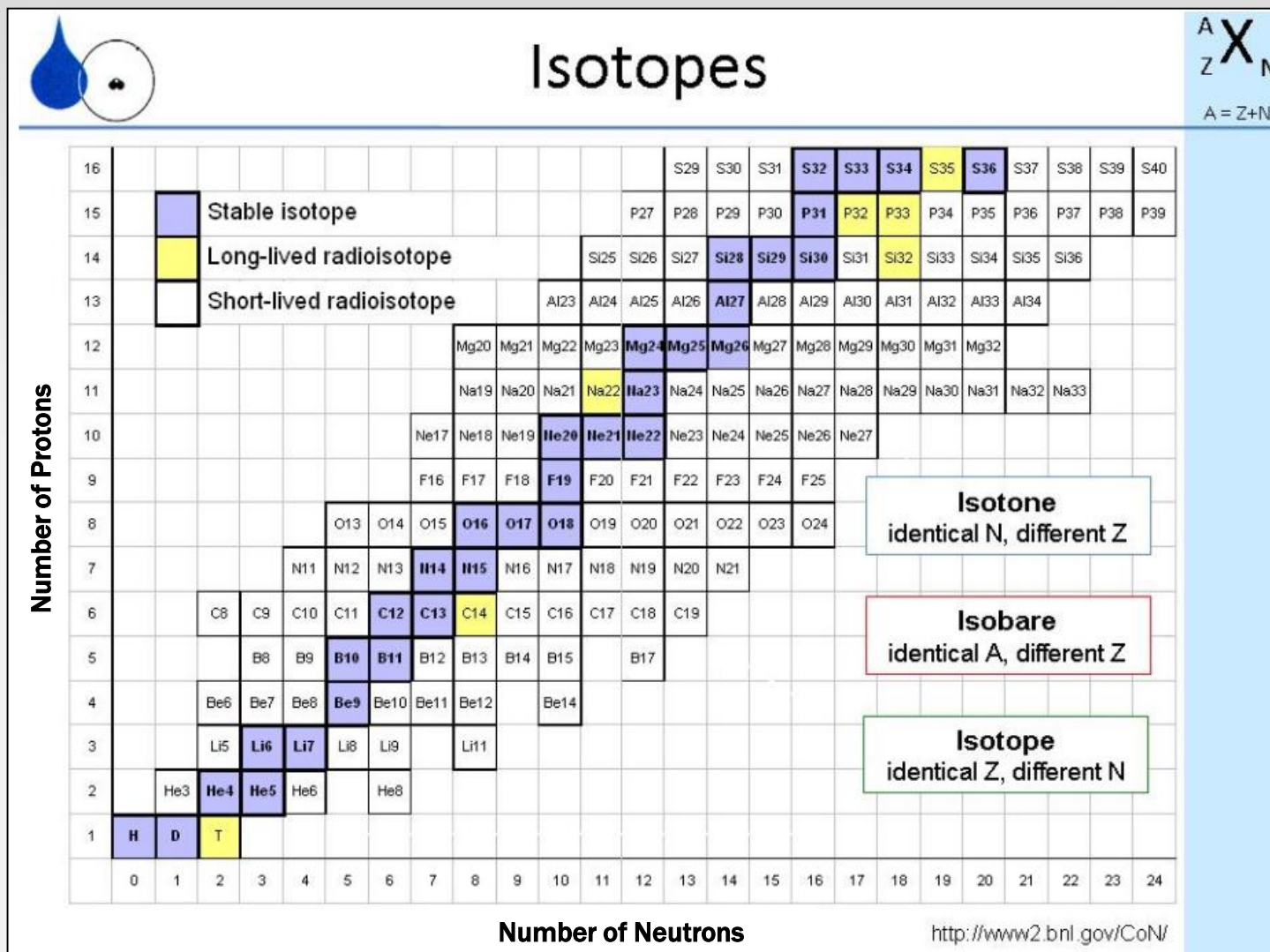


Carbon-14
(6P + 8N)
Atomic Weight = 14
Isotope Mass: 14.003241 u
Abundance: 1 Part Per Trillion
Half-life: $5,730 \pm 40$ Years

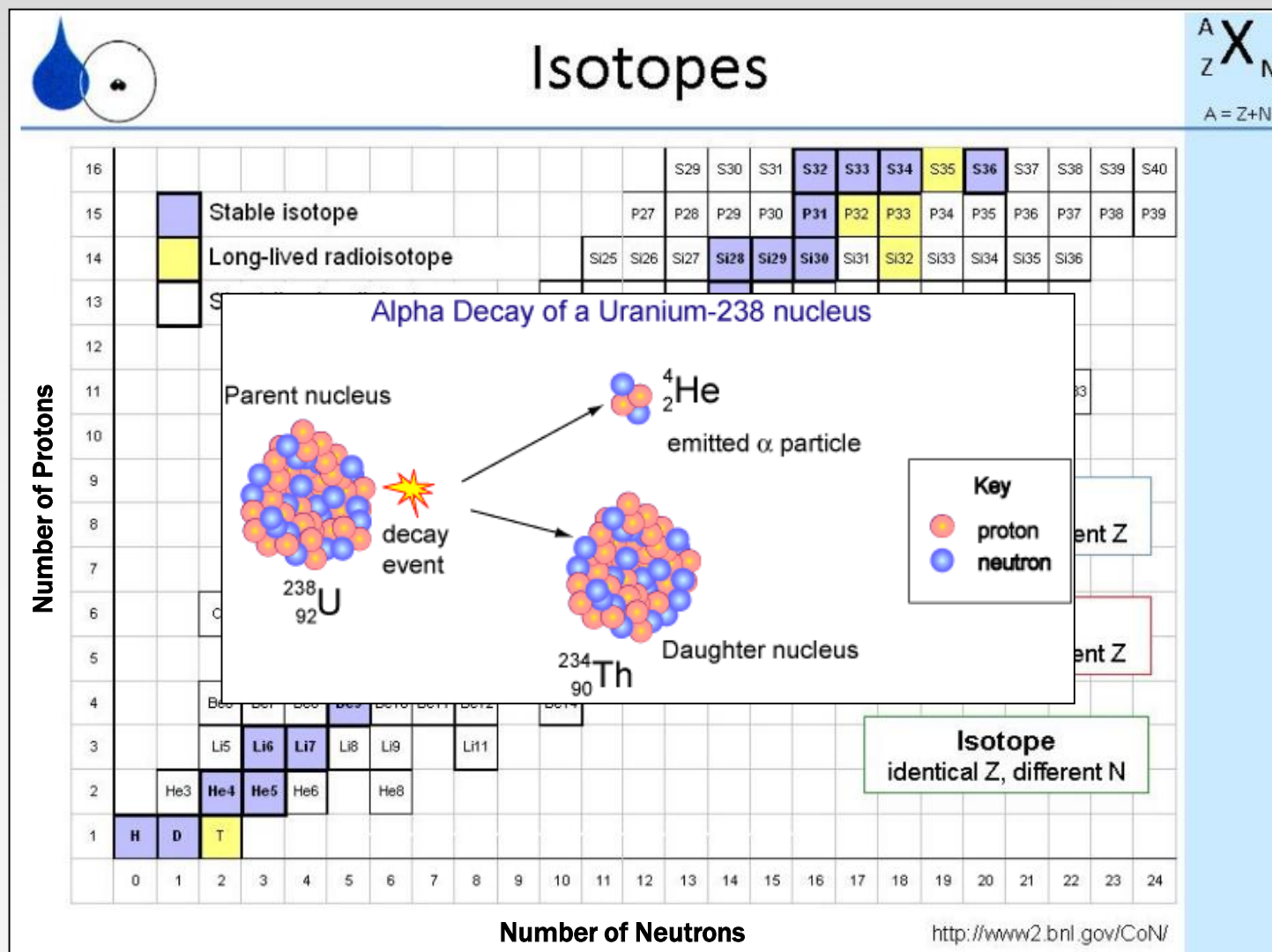




Stable and Unstable Isotopes

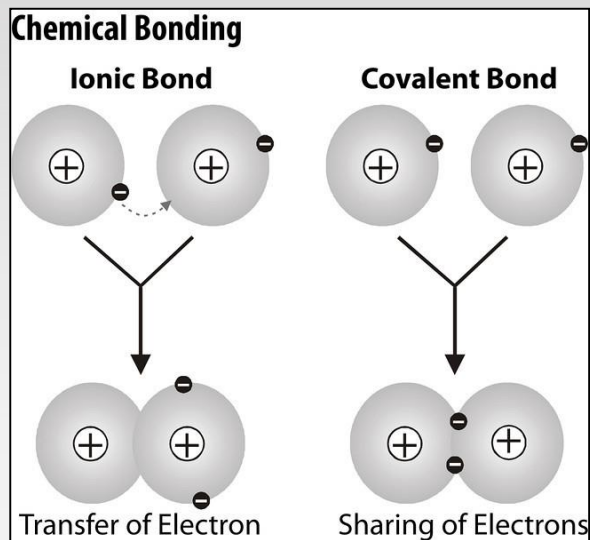


Stable and Unstable Isotopes



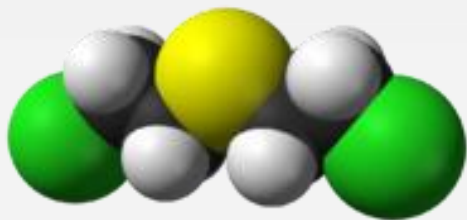


And Back to Atoms... and Molecules

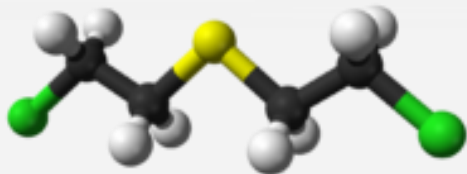


Chemical bonding is all about electrons!

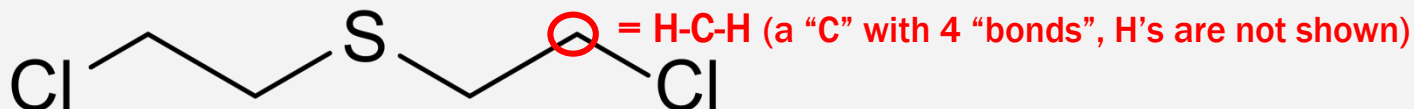
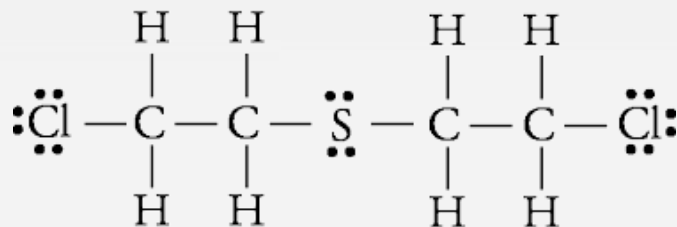
(isotopes do not differ by electrons : chemistry of isotopes of the same element is for practical purposes the same)



=



=





What About Scheduled Chemicals?

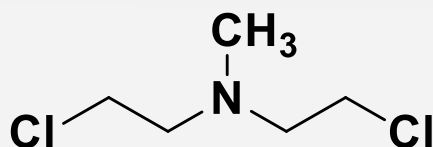
Schedule 1

(CAS registry
number)

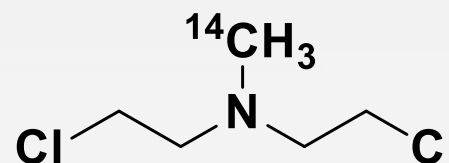
- A. Toxic chemicals:
(6) Nitrogen mustards:

Is it still Schedule 1?

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



Bis(2-chloroethyl)methylamine



Bis(2-chloroethyl)methyl-[¹⁴C]-amine

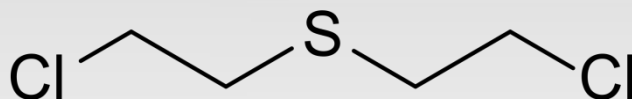
No Assigned CAS Registry Number



Natural Abundance of Stable Isotopes

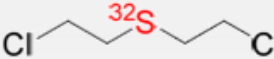
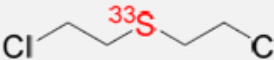
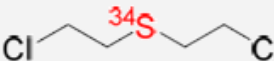
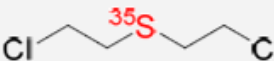

Mustard gas: Bis(2-chloroethyl)sulfide

(505-60-2)



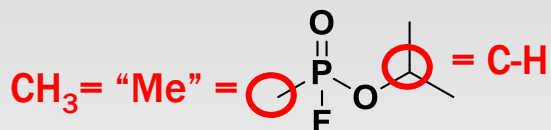
No isotopes indicated

for practical purposes, we assume a sample indicated by this structure contains all isotopes of each element in their natural abundance

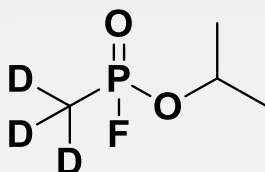
	94.99 %	} sulfur mustard: <i>bis</i> (2-chloroethyl)sulfide as listed within Schedule 1A04 under CAS 505-60-2
	0.75 %	
	4.25 %	
	0.01 %	
	this isotopically labelled form has CAS 6755-76-6	



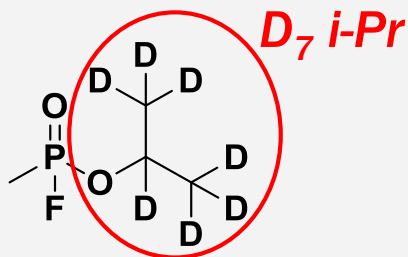
What Schedule Is It?



Isopropyl methylphosphonofluoridate



Isopropyl methyl-d3-phosphonofluoridate



Isopropyl-d7 methylphosphonofluoridate

Schedule 1

(CAS registry
number)

A. Toxic chemicals:

- (1) O-Alkyl ($\leq \text{C}_{10}$, 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)

If CD_3 is considered "not Me", this is unscheduled

Schedule 2

B. Precursors:

Schedule 1A(1) or 2B(4)

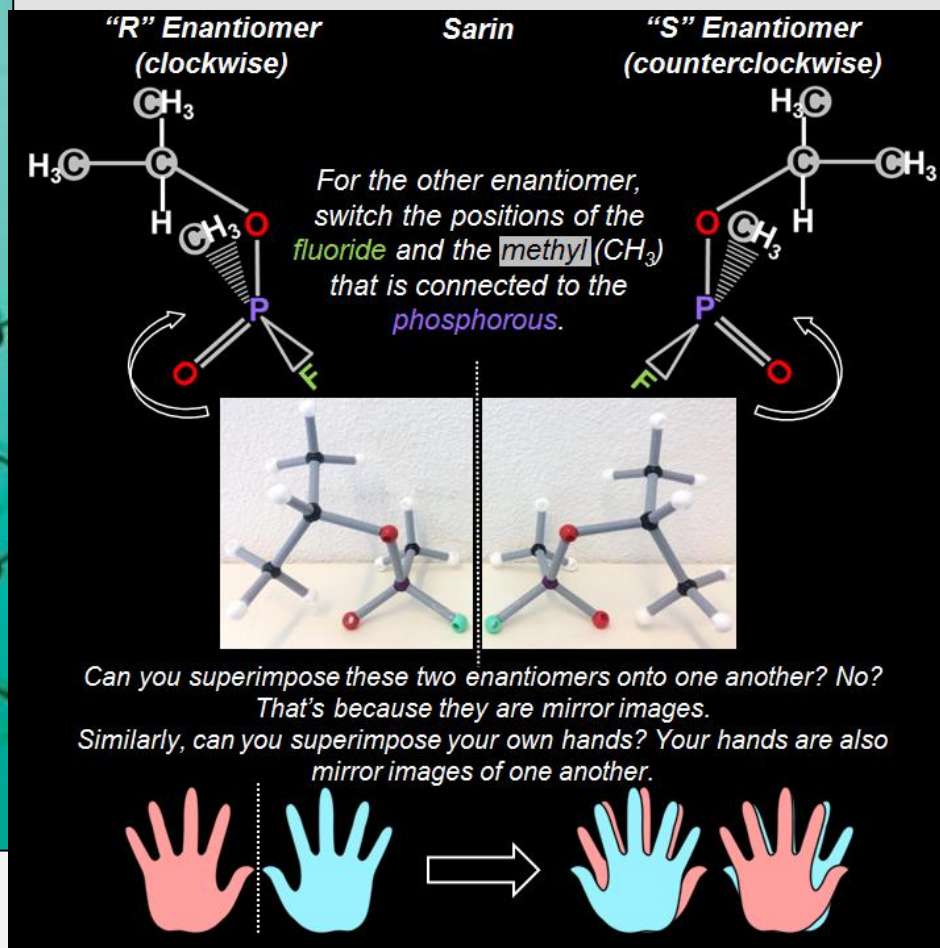
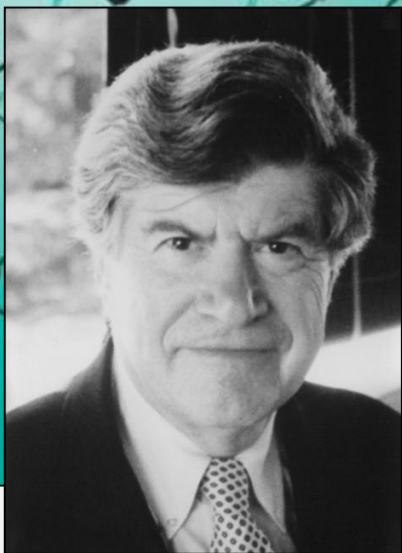
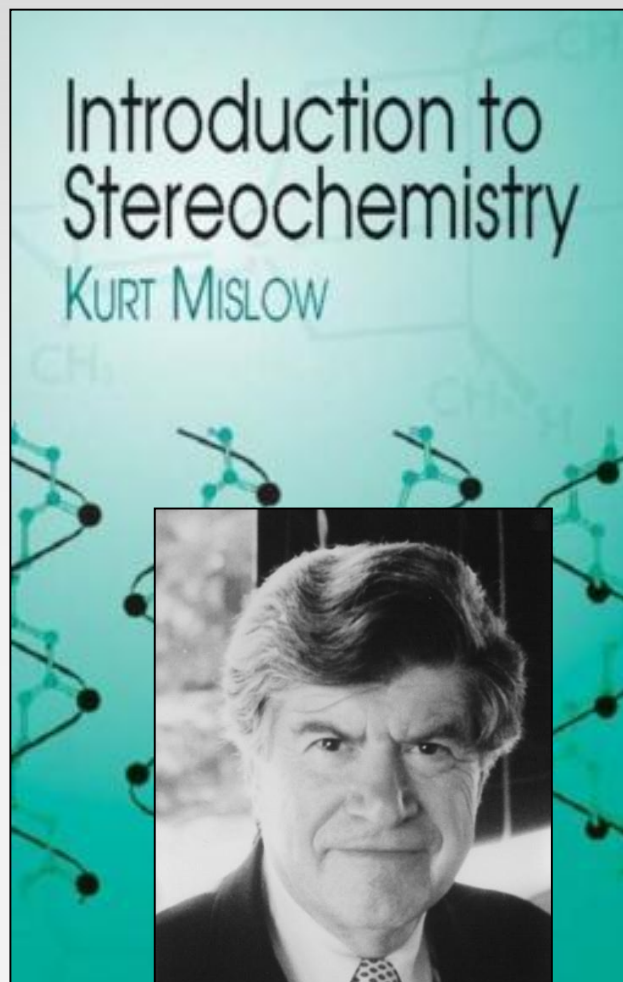
- (4) Chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms,

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

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

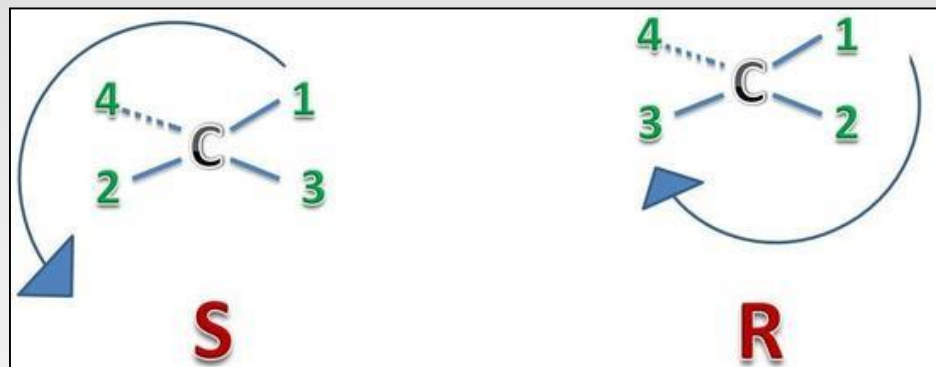
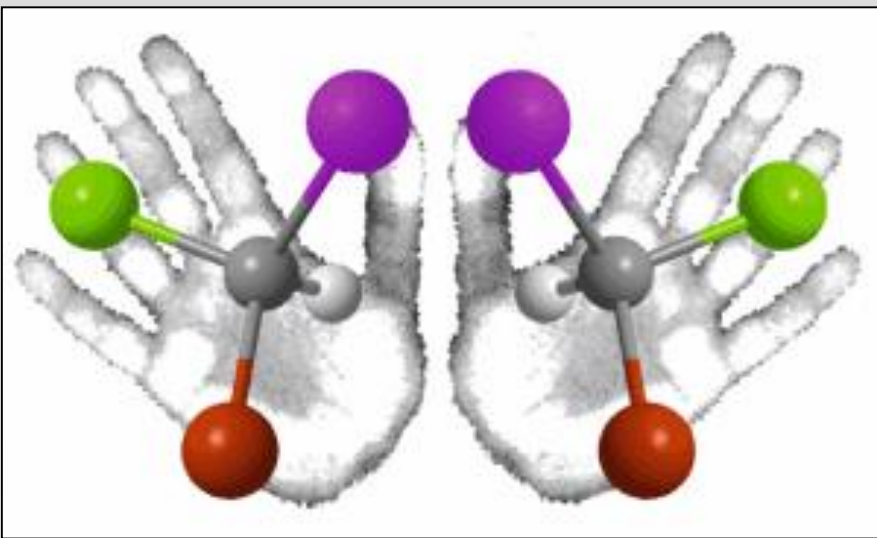


Part 3: Stereoisomers





Three Dimensional Molecular Structure



■ Enantiomers:

- “Mirror image” chemical structures
- Atom with 4 different substituents = “Chiral Center”
- Chemical properties are the same for each enantiomer
- Enantiomers are designated “R” and “S”



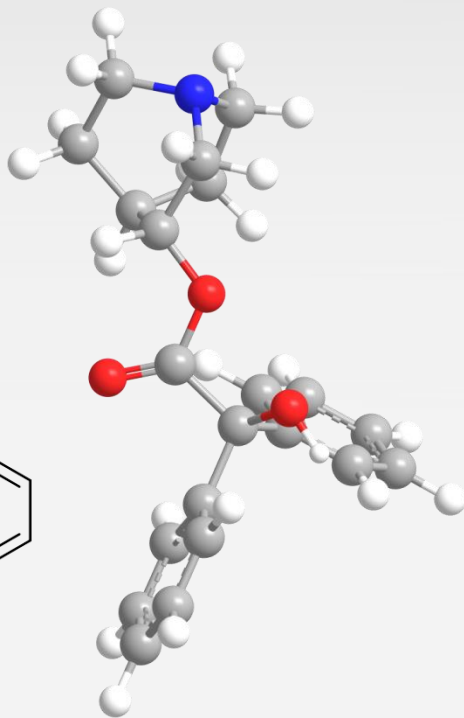
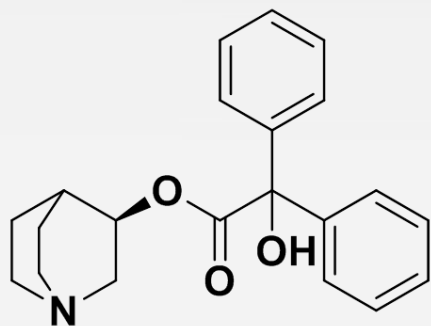
CAS Registry Numbers and Stereoisomers

Schedule 2

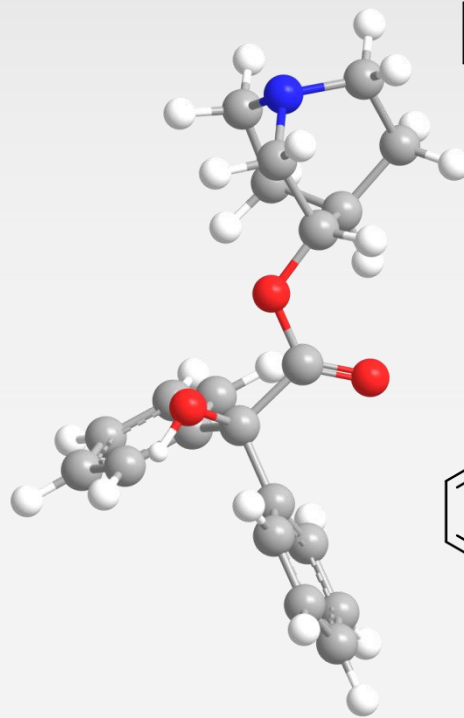
A. Toxic chemicals:

(3) BZ: 3-Quinuclidinyl benzilate (*)

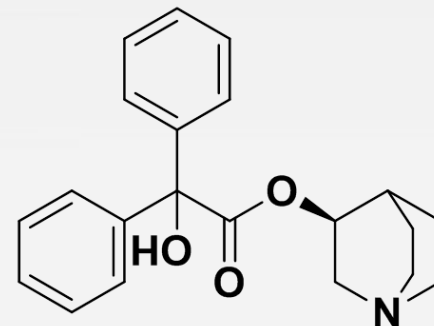
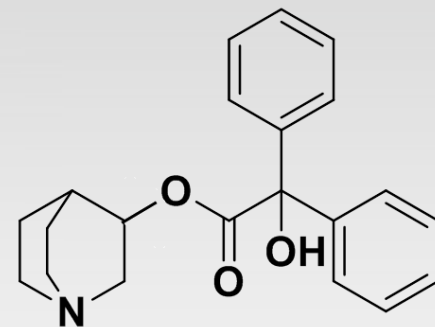
(6581-06-2)



(R)-3-Quinuclidinyl benzilate
CAS Number **62869-69-6**

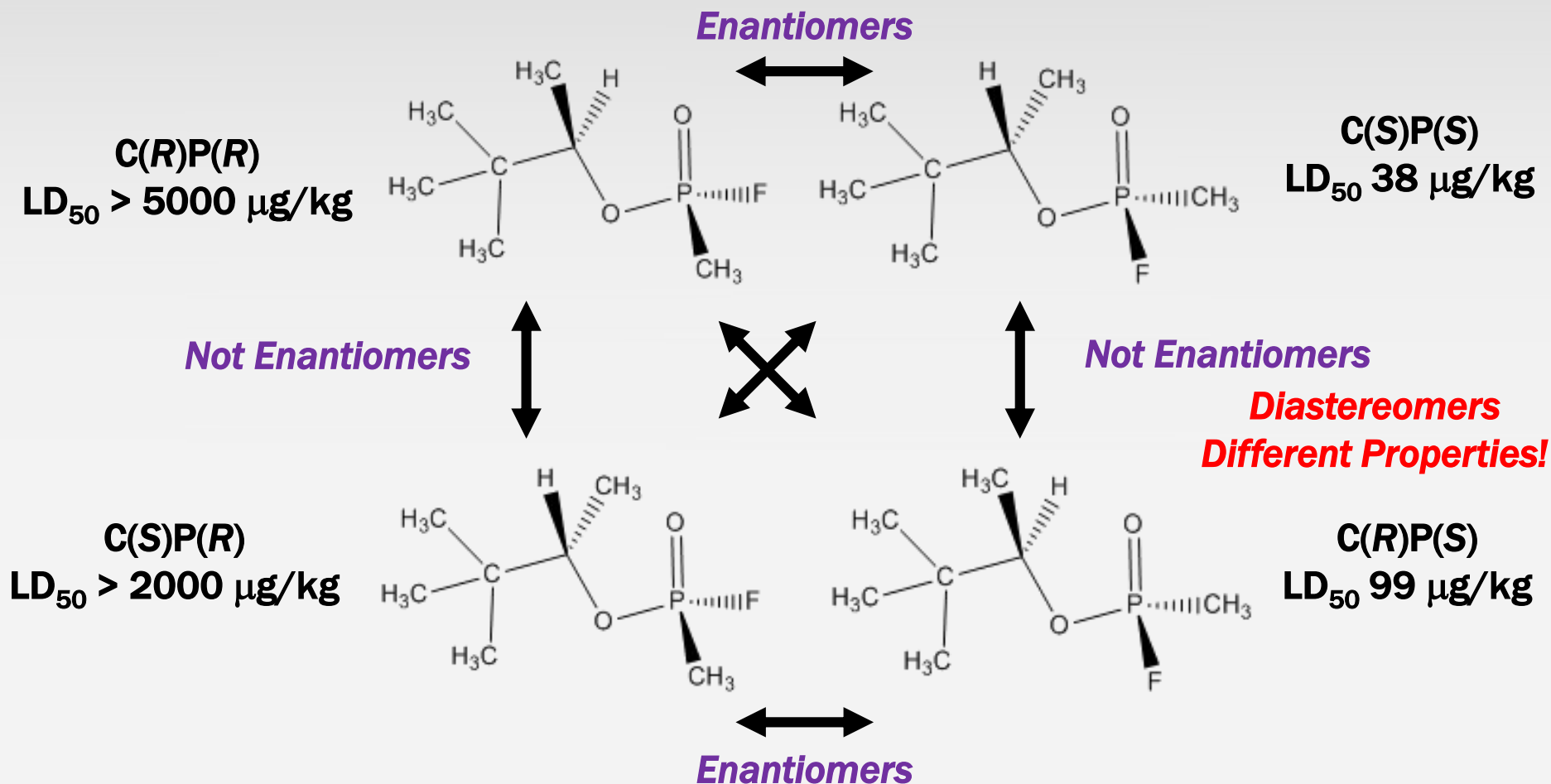


(S)-3-Quinuclidinyl benzilate
CAS Number **62869-68-5**



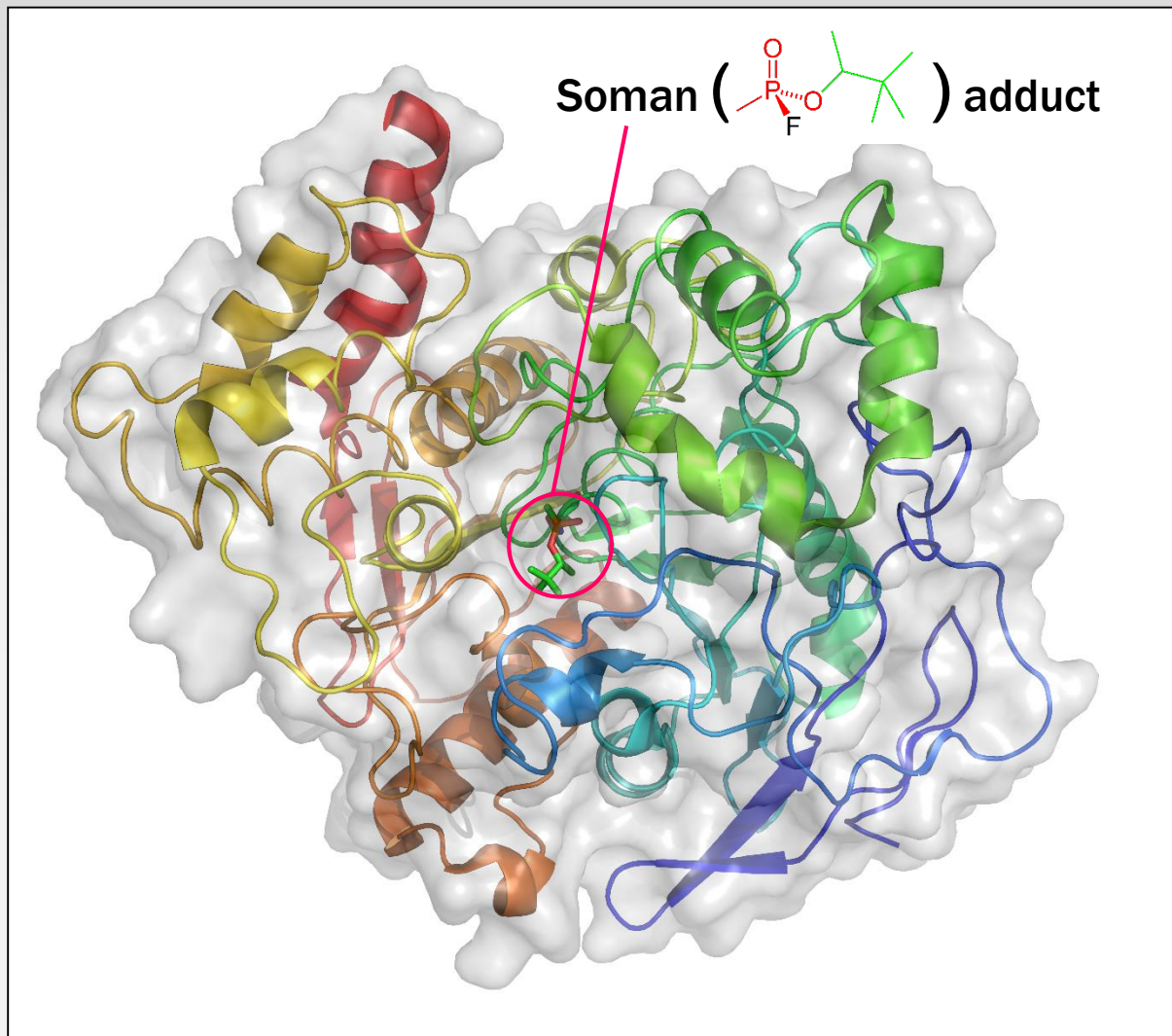


What if There is More than One Chiral Center?





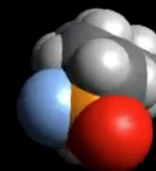
Stereochemistry and Life Processes



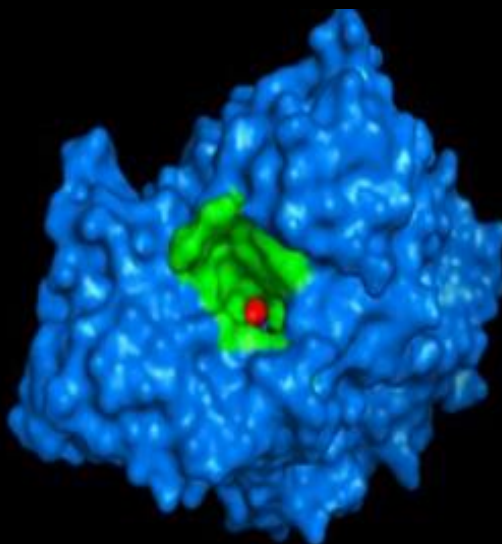
Stereochemistry and Life Processes



C(R)P(R)
LD₅₀ > 5000 μg/kg



C(R)P(S)
LD₅₀ 99 μg/kg



C(S)P(R)
LD₅₀ > 2000 μg/kg



C(S)P(S)
LD₅₀ 38 μg/kg

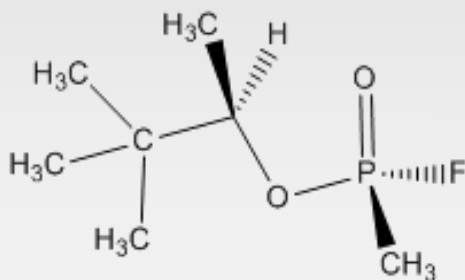




Less Toxic Forms of Soman?

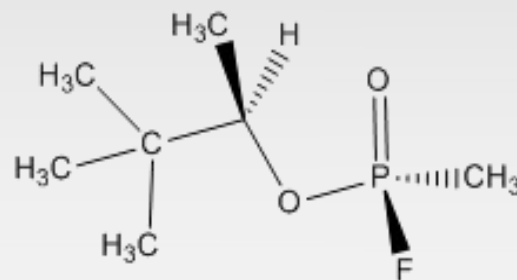
C(R)P(R)

LD₅₀ > 5000 mg/kg



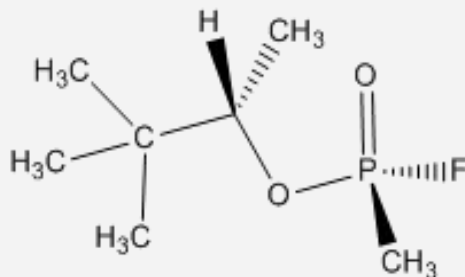
C(R)P(S)

LD₅₀ 99 mg/kg



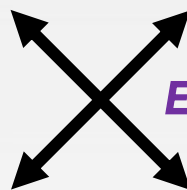
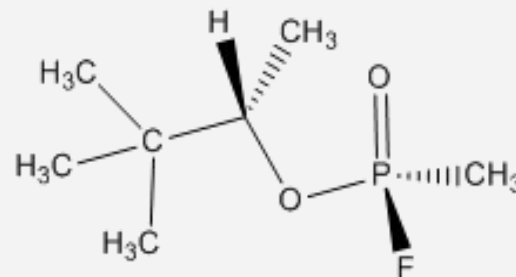
C(S)P(R)

LD₅₀ > 2000 mg/kg

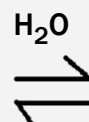
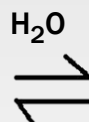


C(S)P(S)

LD₅₀ 38 mg/kg



Enantiomers



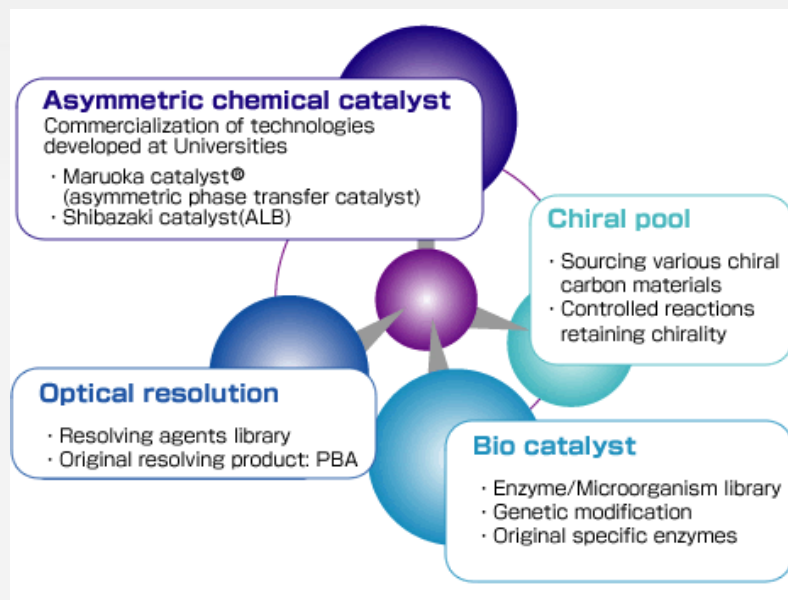


Things to Know About Stereoisomers

- Not all stereoisomers will interconvert
- Under “Achiral” Conditions
 - Chemical synthesis produces racemic mixtures
 - Chemical analysis does not distinguish between enantiomers
- Preparation and isolation of enantiomers
 - Chiral synthesis conditions
 - Biomediated processes
 - Chiral separation conditions

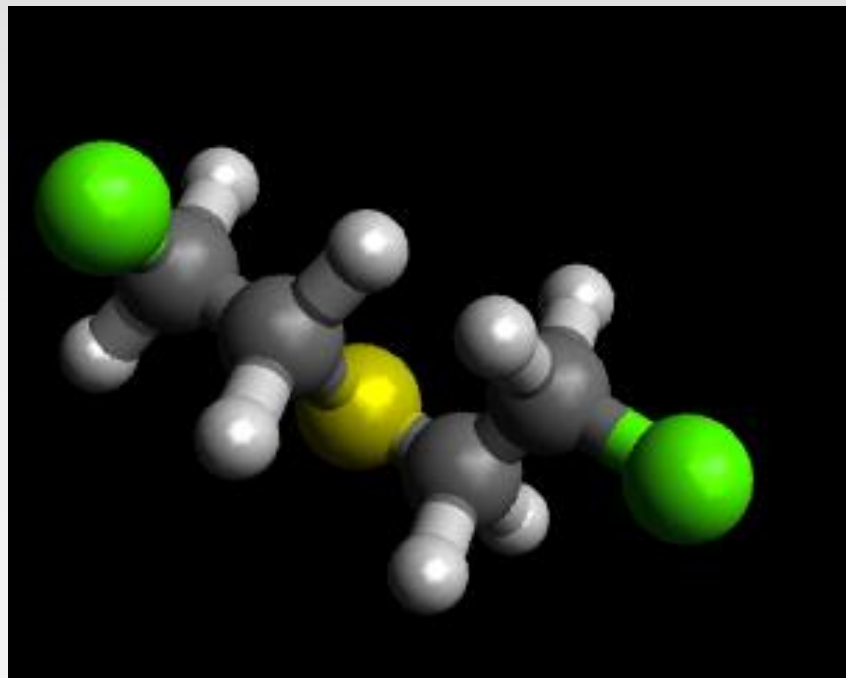
***Sampling and analysis is possible
with appropriate methods and equipment***

***Presence of one might indicate
presence of the other***

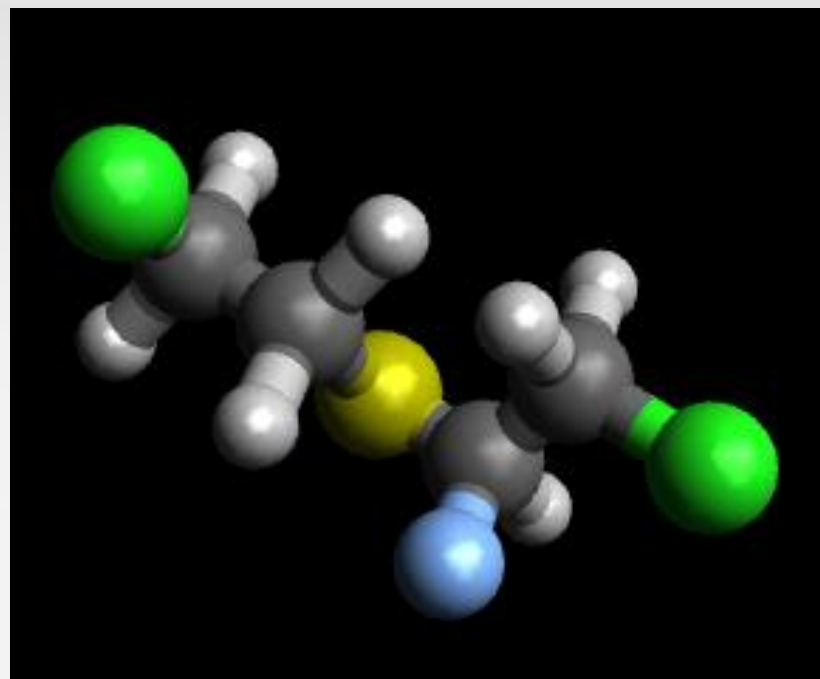




Isotopic Labelling and Stereoisomers (That's Right, They are Not Unrelated!)



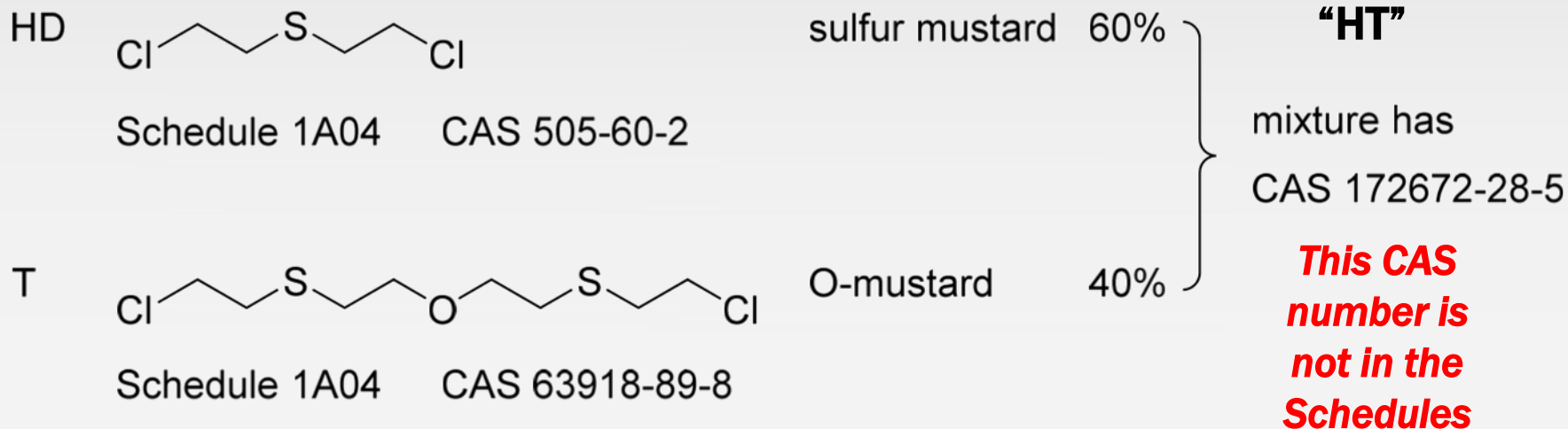
Sulfur Mustard



Replace “H” with “D” on Carbon 2
R or S?



Some Additional Complications: Mixtures!





**RESPONSE TO THE DIRECTOR-GENERAL'S REQUEST TO THE
SCIENTIFIC ADVISORY BOARD TO PROVIDE FURTHER ADVICE
ON SCHEDULED CHEMICALS**

1. RECCOMENDATIONS

- 1.1 The Scientific Advisory Board (SAB) has considered isotopically labelled scheduled chemicals and stereoisomers of scheduled compounds relating to the Convention according to the Director-General's requests (see Appendixes 1 and 2).
- 1.2 **Recommendation 1.** The SAB recommends that the molecular parent structure of a chemical should determine whether it is covered by a schedule entry. This is because:
- (a) it is inappropriate to rely solely upon Chemical Abstracts Service (CAS) numbers to define chemicals covered by the schedules. Although relevant as aids to declaration and verification, CAS numbers should not be used as the means to identify a chemical, or to determine whether a chemical is included in, or excluded from, a schedule;
 - (b) thus, if a chemical is included within a schedule, then all possible isotopically-labelled forms and stereoisomers of that chemical should be included, irrespective of whether or not they have been assigned a CAS number or have CAS numbers different to those shown in the Annex on Chemicals to the Convention. The isotopically labelled compound or stereoisomer related to the parent chemical specified in the schedule should be interpreted as belonging to the same schedule; and
 - (c) this advice is consistent with previous SAB views on this topic.¹
- 1.3 **Recommendation 2.** Inclusion of appropriate analytical data in the OPCW Central Agent Database (OCAD) for isotopically labelled relatives of scheduled compounds where available is recommended.

¹

RG-2/DG.1, dated 28 February 2008, in paragraph 3.5 of its Annex.



How Does This Report Relate to the CWC?

- Each State Party shall adopt the necessary measures to ensure that toxic chemicals and their precursors are only developed, produced, otherwise acquired, retained, transferred, or used within its territory or in any other place under its jurisdiction or control for purposes not prohibited under this Convention. To this end, and in order to verify that activities are in accordance with obligations under this Convention, **each State Party shall subject toxic chemicals and their precursors listed in Schedules 1, 2 and 3 of the Annex on Chemicals, facilities related to such chemicals, and other facilities as specified in the Verification Annex, that are located on its territory or in any other place under its jurisdiction or control, to verification measures as provided in the Verification Annex**



Meeting Obligations

- **To meet these obligations, and to ensure complete and accurate declarations by CWC States Parties to the OPCW, chemicals that fall under Schedules 1, 2, and 3 of the Convention must be clearly identifiable**

Parts VI, VII and VIII to the Convention's Annex on Implementation and Verification set out the relevant requirements



Consistent with Previous Advice from the SAB

■ One issue that the SAB noted in the context of its previous recommendations on salts is the role of the Chemical Abstracts Service (CAS) Registry Numbers indicated in the schedules of chemicals. The SAB has come to the view that, while the CAS Registry Numbers are a useful aid to identification, they were intended as specific identifiers of scheduled chemicals. There appears to be a question among States Parties about whether these numbers have a regulatory value. The SAB would like to caution against such a view, because **there is not necessarily a one-to-one relationship between CAS Registry Numbers and chemical structures.** While these numbers are useful in the identification of chemical compounds, this usefulness should not lead to the assumption that they should have any regulatory power within the context of the Convention. At the same time, it could be helpful if the OPCW Declaration Handbook were to provide references to the various CAS numbers that are related to an entry in the schedules (for example, for different isomers of a scheduled chemical and for mixtures containing a scheduled chemical).

RC-2/DG.1, dated 28 February 2008, in paragraph 3.5 of the Annex

Declarations Handbook does provide references and examples as suggested



Handbook on Chemicals

Chemical name: Cyclohexyl methyl-d₃-phosphonofluoridate

Schedule: 1A01

CAS RN:

HS code: 2845.90

Key: (108-93-0)-M1A1(D3)

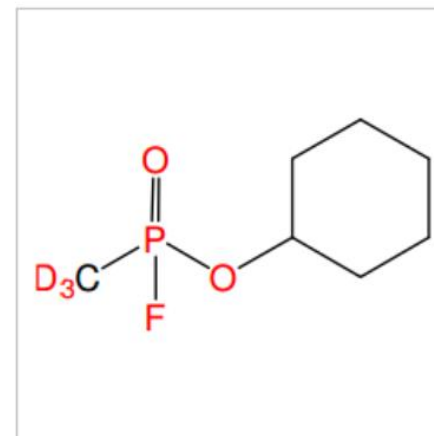
Molecular formula: C₇H₁₁D₃FO₂P

CAS Index Name: Phosphonofluoridic acid, methyl-d₃-, cyclohexyl ester

IUPAC name: Cyclohexyl methyl-d₃-phosphonofluoridoate

Synonyms: O-Cyclohexyl trideuteriomethylphosphonofluoridate

O-Cyclohexyl methyl-d₃-phosphonofluoridate





Moving Forward

- **Encourage sharing of this SAB advice with National Authorities**
- **Continue current practices in regard to declarations handbook and OCAD**



ORGANISATION FOR THE
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More to Come on Isotopes and Chemical Weapons



SAB Workshop #1: Chemical Forensics 20 – 22 June 2016, Helsinki, Finland
(report forthcoming)

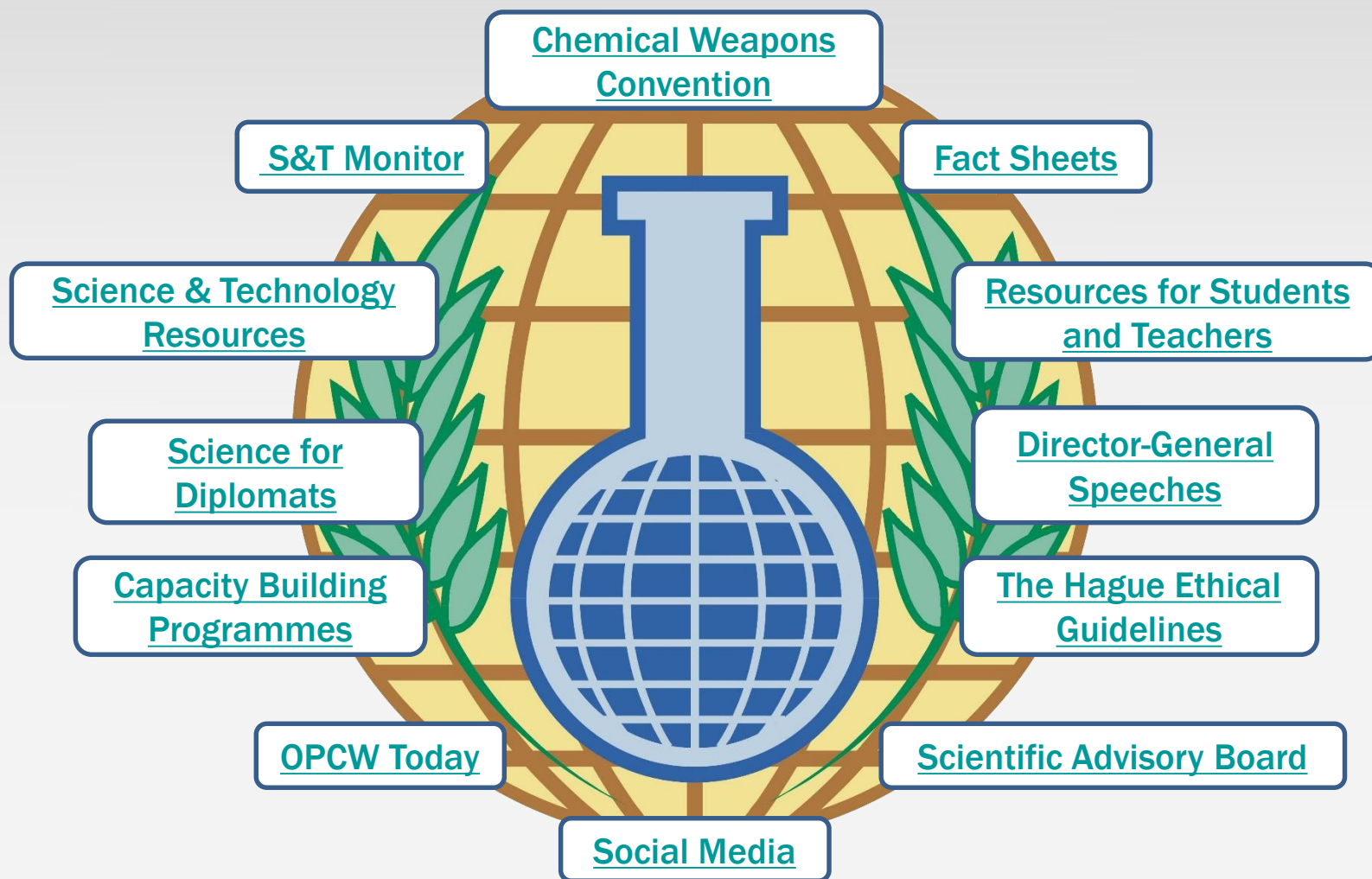


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OPCW Science and Technology Related Resources

<https://www.opcw.org/special-sections/science-technology/science-technology-resources/>





OPCW Science and Technology Related Resources

<https://www.opcw.org/special-sections/science-technology/science-technology-resources/>

S&T M

Science & Technology
Resources

Science for
Diplomats

Capacity Building
Programmes

OPCW

Sheets

Resources for Students
and Teachers

Director-General
Speeches

The Hague Ethical
Guidelines

Scientific Advisory Board



The OPCW Science & Technology Monitor

Volume 3 Number 3

A sampling of Science & Technology
Relevant to the Chemical Weapons Convention

6 July 2016

In this Issue



Image courtesy of Brian Jones

**Medicines, Drugs
and Incapacitants:
CNS Acting
Chemicals**



Image courtesy of Jiaqi Ma

**Artificial
Intelligence**



Image © OPCW

**SAB, ABEO and
OPCW Day reports**

Welcome

Welcome to the OPCW Science and Technology Monitor, an occasional bulletin providing updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues (and more) can be found on the [Science and Technology section of the OPCW website](#).



The Mars rover Sojourner (left) and a Micro Air Vehicle (right) going on reconnaissance missions near The Dunes (Mars) and China Lake (Earth).
Images courtesy of NASA and US Navy

This third issue of 2016 comes on the 19th anniversary of the day that [Mars rover Sojourner became the first man-made vehicle to travel across the surface of another planet](#). Sojourner was designed to operate for one week, yet operated and produced data for nearly three months. Today on Earth, [autonomous vehicles](#) (many larger and equipped with more instruments than Sojourner) are becoming more and more commonplace. In the spirit of the Mars rovers, autonomous systems that can collect and transmit information (including from environments dangerous to humans) open up many [opportunities for scientific applications](#) and even for [detecting chemical weapons](#)!

The S&T Puzzle

Congratulations go out to our first puzzle winner from OPCW's International Cooperation and Assistance Division (ICA). One of the ICA's interns took the prize on what he described as a "befuddling task". Puzzle statistics now stand at: VER 6, CTBTO 5, OSP 2, OCS 1, INS 1 and ICA 1. The answers can be found on the last page!

For this edition of the puzzle, we challenge you to recognize the "Sounds of the OPCW". The first person to correctly identify the five below wins the prize: your choice of requesting a featured topic, designing a puzzle or receiving a beverage hand selected by the Science Policy Adviser. Send answers to scitech@opcw.org. Good luck!



- [Sound 1](#)
- [Sound 2](#)
- [Sound 3](#)
- [Sound 4](#)
- [Sound 5](#)



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Science Engagement Pond Mission 2016





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Science Engagement Pond Mission 2016

Working together for a world free of chemical weapons





Science and Technology For Diplomats Upcoming Events

- October 2016 (On the margins of EC-83, to be confirmed)
 - **Science for Diplomats: SAB Reports from Workshops on Chemical Forensics and Chemical Warfare Agent Toxicity**
- December 2016 (at CSP-21, to be confirmed)
 - **Briefing on 2016 SAB activities**
 - **Science for Diplomats: SAB Report on Sample Handling and Storage**
- **For more information on S&T from OPCW**

SciTech@OPCW.org (email)

@OPCW_ST (Twitter)

www.opcw.org/special-sections/science-technology/

