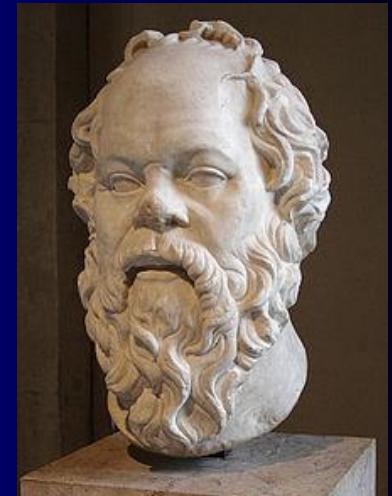


# Introduction to PLASMA PHYSICS

Scio me nihil scire



(„Vím, že nic nevím.“

I know that I know nothing)

Consistency of the universe

Socrates (470–399 BC)

# Introduction to PLASMA PHYSICS

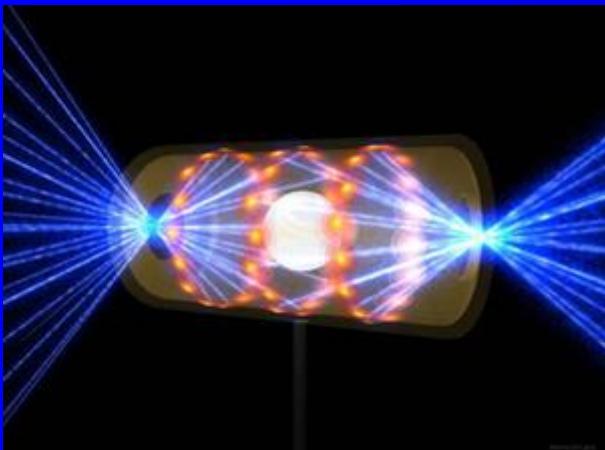
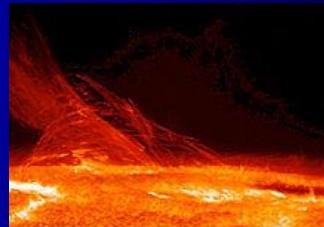
UFP 1A ZS 2024

Andromeda composite

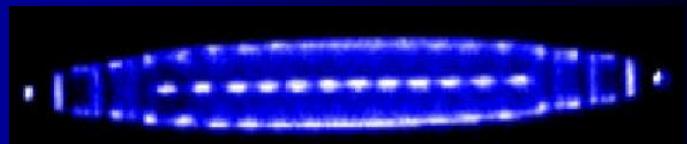
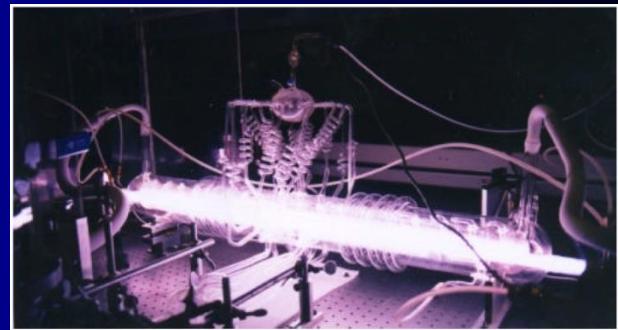
Prof. J. Glosík  
KFPP MFF UK



Burning Match Stick



**Fusion in a flash.** At the National Ignition Facility (NIF) at Lawrence Livermore National Lab, 192 powerful lasers blast a BB-sized fuel pellet inside a metallic cylinder to generate nuclear fusion.



**This presentation is only for students attending the lectures**

**INTRODUCTIO TO PLASMA PHYSICS at MFF UK,**

**Not for public use. Preliminary version without references.**

**Language – Czech, English, Slovak (česky, slovensky, anglicky) ... in approximation ... ?**

## Recommended literature :



**Úvod do fyziky plazmatu**  
**(Introduction to Plasma Physics)**

Francis F. Chen  
Academia Praha 1984 (Plenum press 1974)

E

**Základy fyziky plazmy**  
Viktor Martišovič  
Bratislava 2004  
Učebný text pre 3. ročník magisterského štúdia

Cz

**Fundamentals of plasma physics**  
J. A. Bittencourt  
Springer,  
Third Edition 2004

E

**Physics of Ionized Gases**  
Boris M. Smirnov  
John Wiley&Sons 2001

E

**Základy klasické a kvantové fyziky plazmatu**

„Velký Kracík“  
J.Kracík, B. Šesták a L. Aubrecht  
Academia Praha 1974

Cz

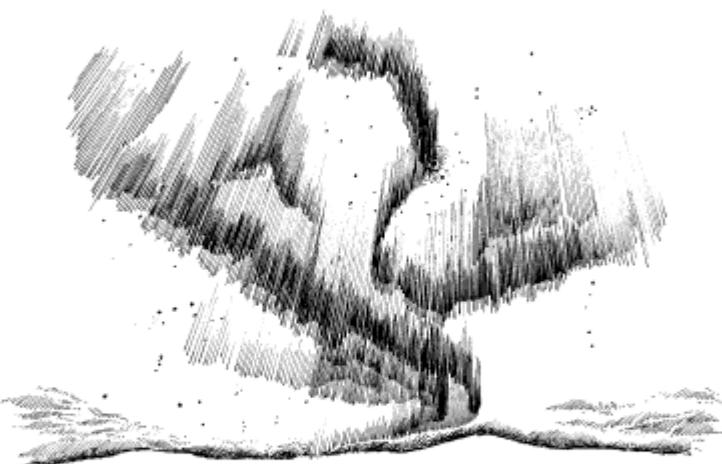
**Fyzika plazmatu**  
J.Kracík, J. Tobiáš  
Academia, Praha 1966  
„Malý Kracík“

Cz

**ASTRONOMIE A FYZIKA NA PŘELOMU TISÍCILETÍ**  
Pod vedením Petra Kulhánka  
Aldebaran Group for Astrophysics, 2004

Cz

# Úvod do teorie plazmatu

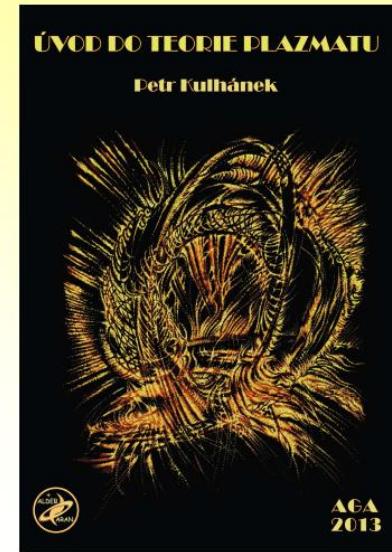


Petr Kulhánek

AGA 2020

- V textu byly použity některé obrázky a text z knihy:

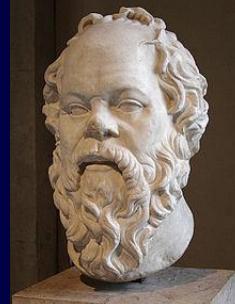
P. Kulhánek, Úvod do teorie plazmatu, AGA 2011, Praha.





Information ...???

# Scio me nihil scire



( I know that I know nothing)

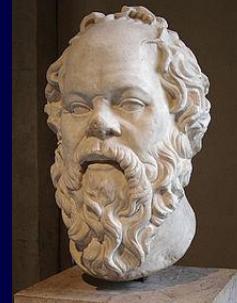


1TB

## THE EXPERTS SPEAK<sup>†</sup>

- “There is not the slightest indication that [nuclear] energy will ever be obtained” — *Albert Einstein, 1932*
- “Anyone who expects a source of power from the transformation of these atoms is talking moonshine.” — *Ernest Rutherford, 1933*
- “A few decades hence, [when controlled fusion is achieved], energy will be free — just like the unmetered air.” — *John von Neumann, 1956*
- “Radio has no future.” — *Lord Kelvin, 1897*
- “I think there is a world market for about five computers.” — *Thomas J. Watson, 1943*
- Where a calculator like ENIAC is equipped with 18,000 vacuum tubes and weighs 30 tons, computers in the future may have only 1,000 vacuum tubes and perhaps only weigh  $1\frac{1}{2}$  tons.” — *Popular Mechanics, March 1949*
- “640k ought to be enough for anybody.” — *Bill Gates, 1981*

<sup>†</sup> C. Cerf and V. Navasky, Villard, New York, 1998



# Information ....



**Scio me nihil scire**

(„Vím, že nic nevím.“      I know that I know nothing)



★★★★★ 4,5 640k

SanDisk Ultra Dual Drive Luxe 1TB

Flash disk 1000 GB - USB 3.2 Gen 1 (USB 3.0), konektor USB-C, rychlosť zápisu až 20 MB/s, rychlosť čítania až 150 MB/s.



## THE EXPERTS SPEAK<sup>†</sup>

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# Plasma

History of the term “**plasma**” In the mid-19th century the Czech physiologist **Jan Evangelista Purkyně** introduced use of the Greek word plasma (meaning “formed or molded”) to denote the clear fluid which remains after removal of all the corpuscular material in blood.

Half a century later, the American scientist **Irving Langmuir proposed** in **1922** that the electrons, ions and neutrals in an ionized gas could similarly be considered as corpuscular material entrained in some kind of fluid medium and called this entraining medium **plasma**. However it turned out that unlike blood where there really is a fluid medium carrying the corpuscular material, there actually is no “fluid medium” entraining the electrons, ions, and neutrals in an ionized gas. Ever since, plasma scientists have had to explain to friends and acquaintances that they were not studying blood!

Jan Evangelista Purkyně was a Czech anatomist and physiologist. In 1839, he coined the term protoplasm for the fluid substance of a cell. He was one of the best known scientists of his time. [Wikipedia](#)

Purkyně also introduced the scientific terms plasma (for the component of blood left when the suspended cells have been removed) and protoplasm (the substance found inside cells.)

## Definition of a plasma

Although a plasma is loosely described as an electrically neutral medium of positive and negative particles, a more rigorous definition requires three criteria to be satisfied:

### The plasma approximation:

Charged particles must be close enough together that each particle influences **many nearby charged particles**, rather than just the interacting with the closest particle (these collective effects are a distinguishing feature of a plasma). The plasma approximation is valid when the number of electrons within the sphere of influence (called the *Debye sphere* whose radius is the **Debye (screening) length**) of a particular particle is **large**. The average number of particles in the Debye sphere is given by the **plasma parameter,  $\Lambda$** .

### Bulk interactions:

The Debye screening length (defined above) is short compared to the physical size of the plasma. This criterion means that interactions in the bulk of the plasma are more important than those at its edges, where boundary effects may take place.

### Plasma frequency:

The electron plasma frequency (measuring **plasma oscillations** of the electrons) is large compared to the electron-neutral collision frequency (measuring frequency of collisions between electrons and neutral particles). When this condition is valid, plasmas act to shield charges very rapidly (**quasineutrality** is another defining property of plasmas).

# Charged Particle Trajectories Are Different In Plasmas

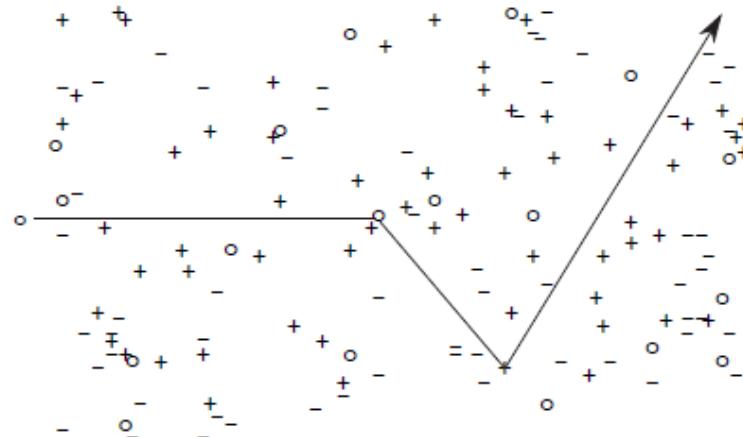


Figure 3: The trajectory of a neutral particle in a partially ionized gas exhibits “straight-line” motion between abrupt atomic collisions. The typical distance between neutral particle collisions is called the collision “**mean free path**.” Symbols: neutrals (circles), electrons (minus signs) and ions (plus signs).

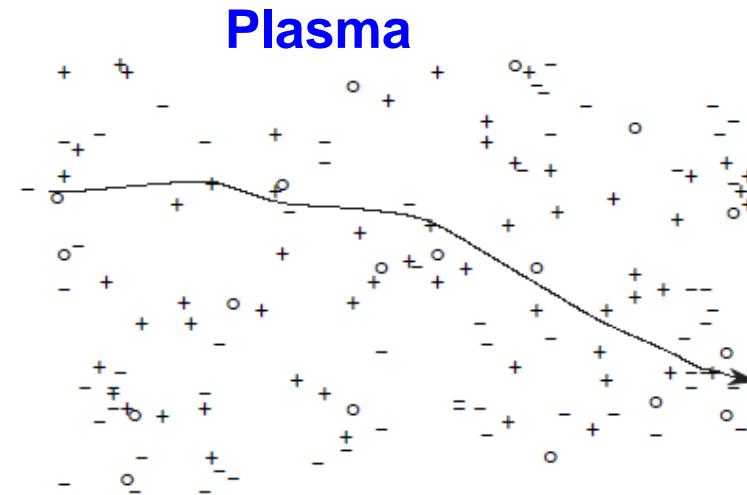


Figure 4: The trajectory of a “test” electron in a plasma exhibits continuous small-angle Coulomb collisional scatterings of its direction of motion. The “**collision length**” is the exponential decay length over which an average charged particle in a plasma loses its initially directed momentum.

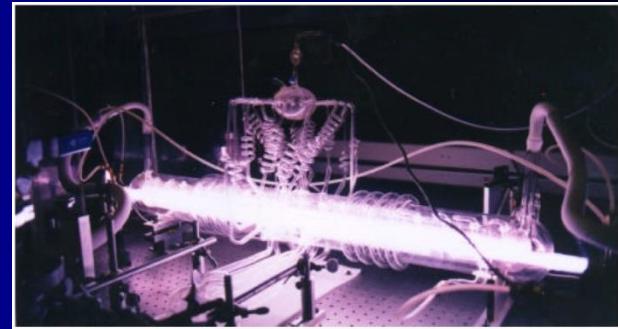
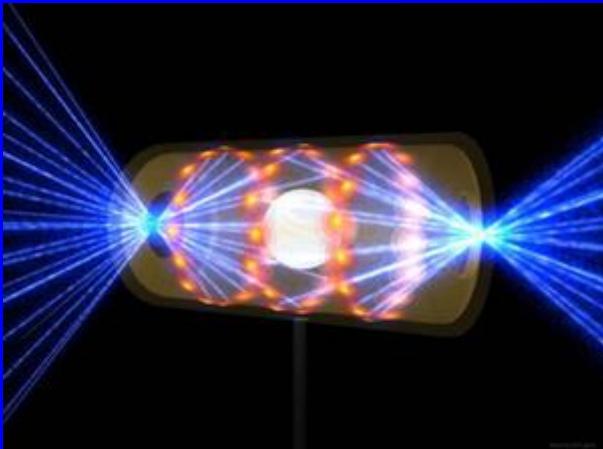
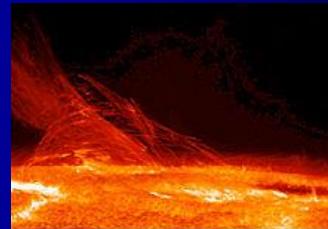
# Introduction to PLASMA PHYSICS

Prof. J. Glosík  
KFPP MFF UK

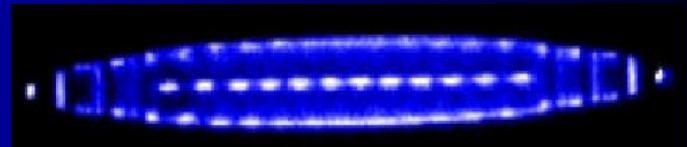
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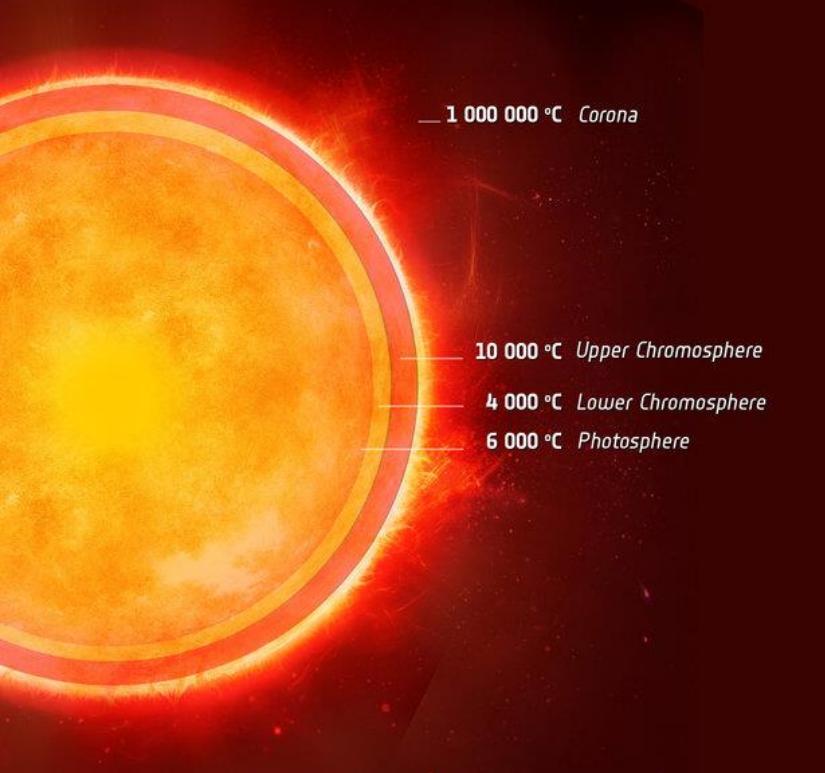


Burning Match Stick

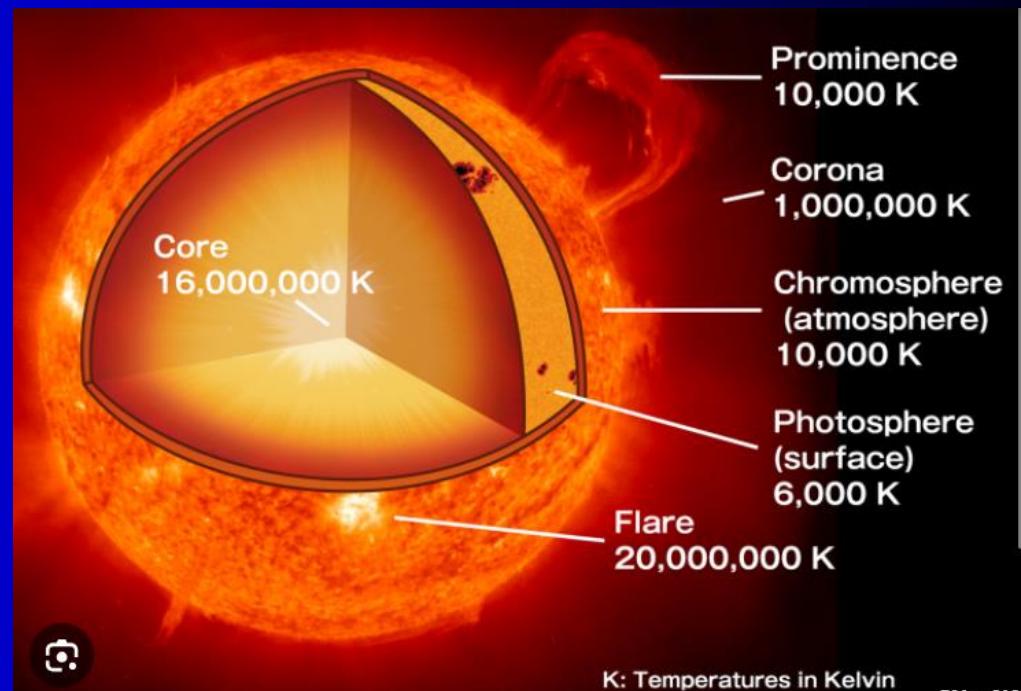


**Fusion in a flash.** At the National Ignition Facility (NIF) at Lawrence Livermore National Lab, 192 powerful lasers blast a BB-sized fuel pellet inside a metallic cylinder to generate nuclear fusion.

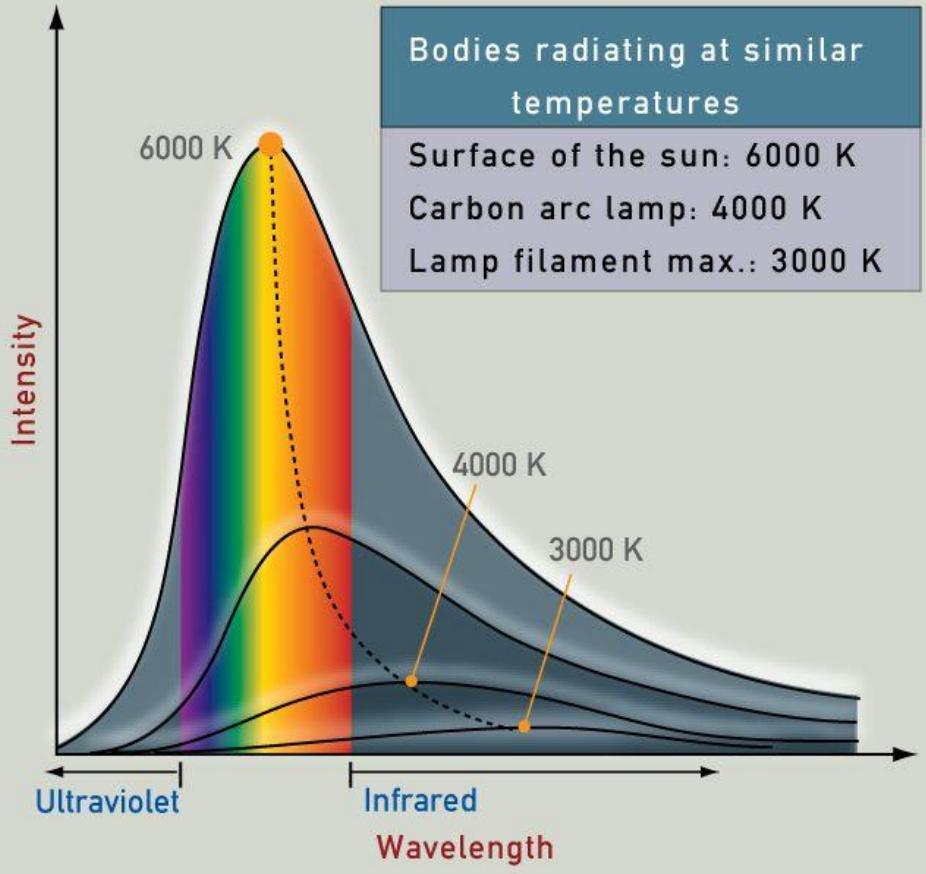




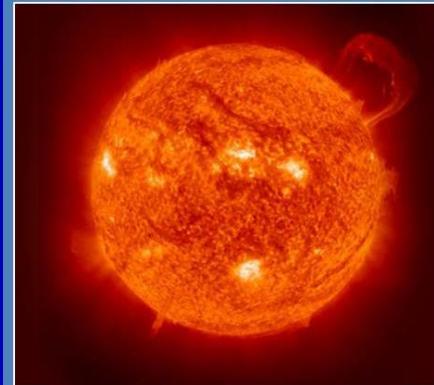
## Temperature of the Sun ???



# Blackbody Radiation Curves



SURFACE TEMPERATURE  
OF THE SUN & EARTH

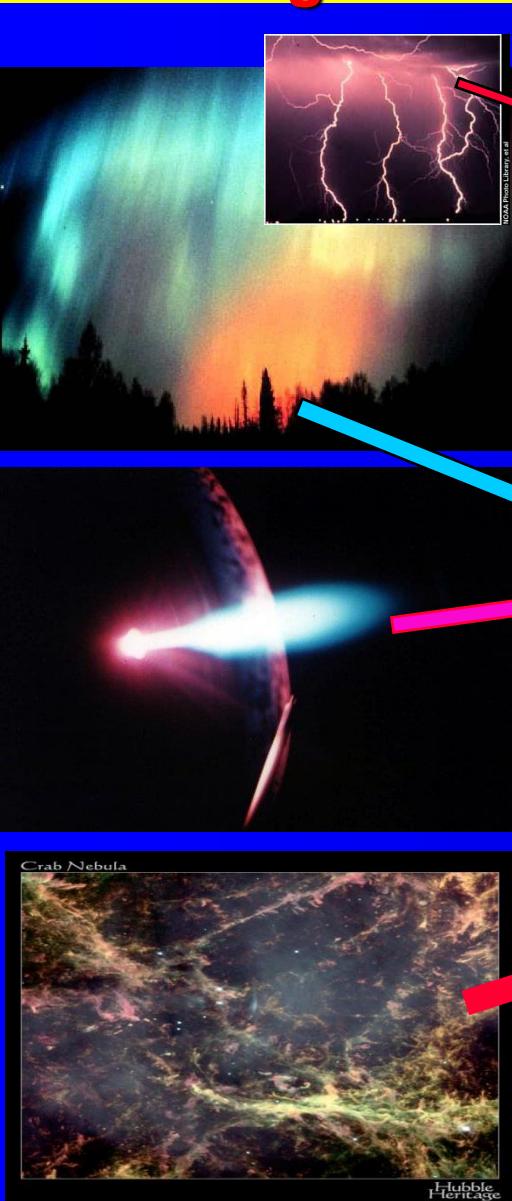


6,000K (5,727°C or 10,340°F)



288K (15°C or 59°F)

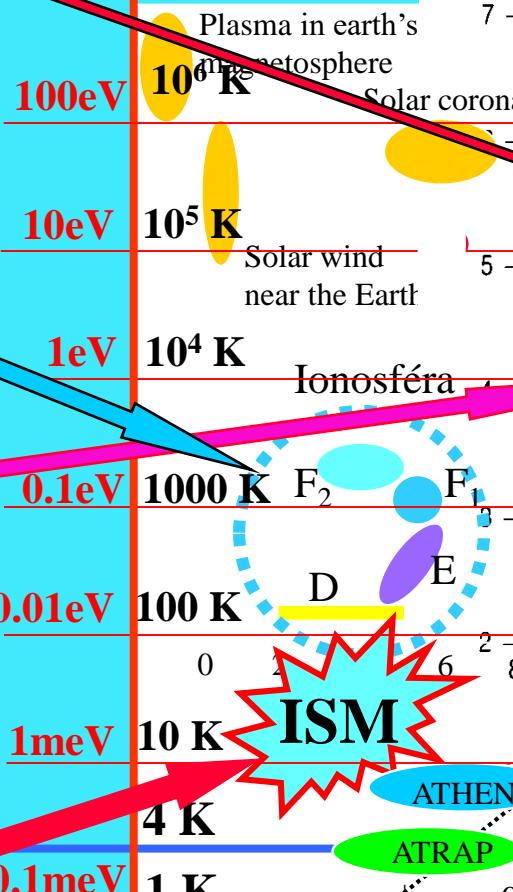
# Temperatures and energies



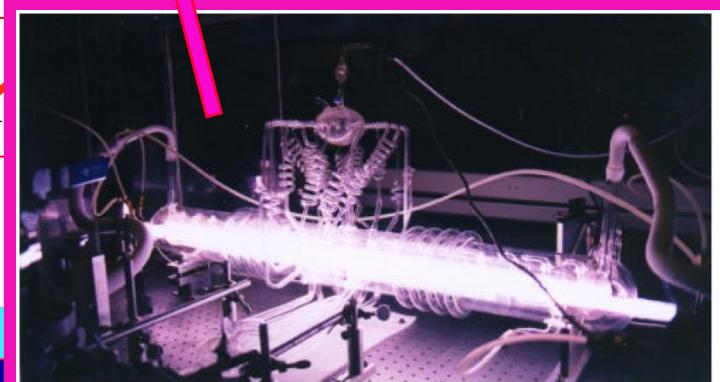
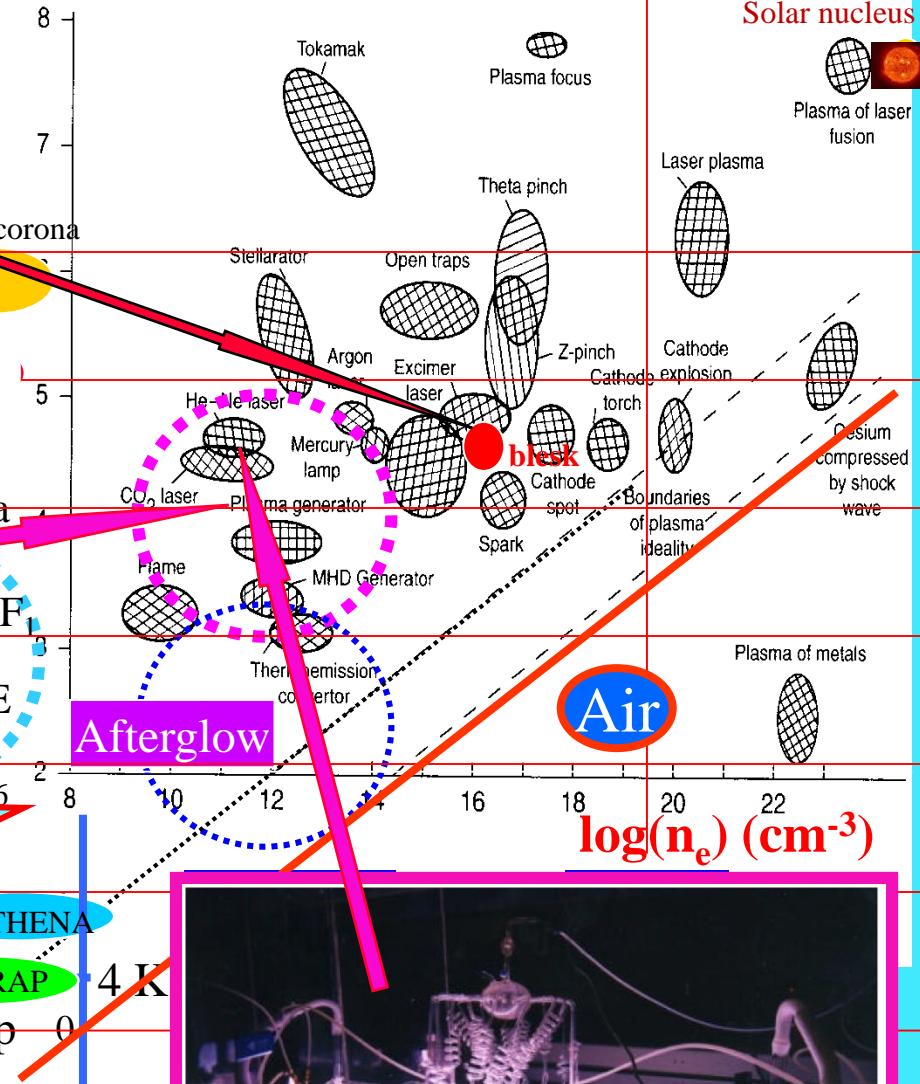
$$E \leftrightarrow kT$$

$$1\text{eV} \sim 11\,604.505 \text{ K}$$

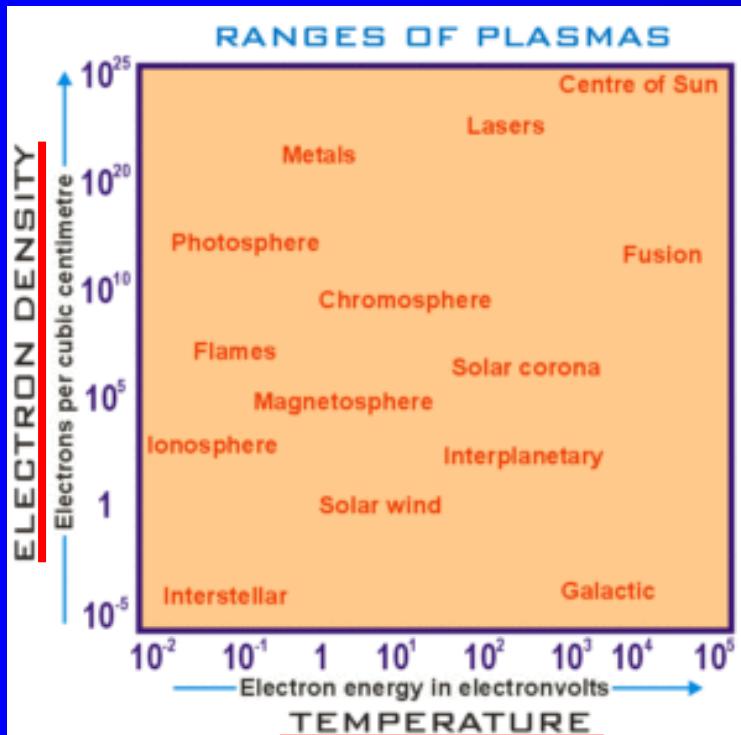
$$1\text{K} \sim 9 \times 10^{-5} \text{ eV}$$



$\log T_e (\text{K})$



Not actualized, approximation



## Ranges of plasma parameters

Density increases upwards, temperature increases towards the right. The free electrons in a metal may be considered an electron plasma. Plasma parameters can take on values varying by many orders of magnitude, but the properties of plasmas with apparently disparate parameters may be very similar (see plasma scaling). The following chart considers only conventional atomic plasmas and not exotic phenomena like quark gluon plasmas:

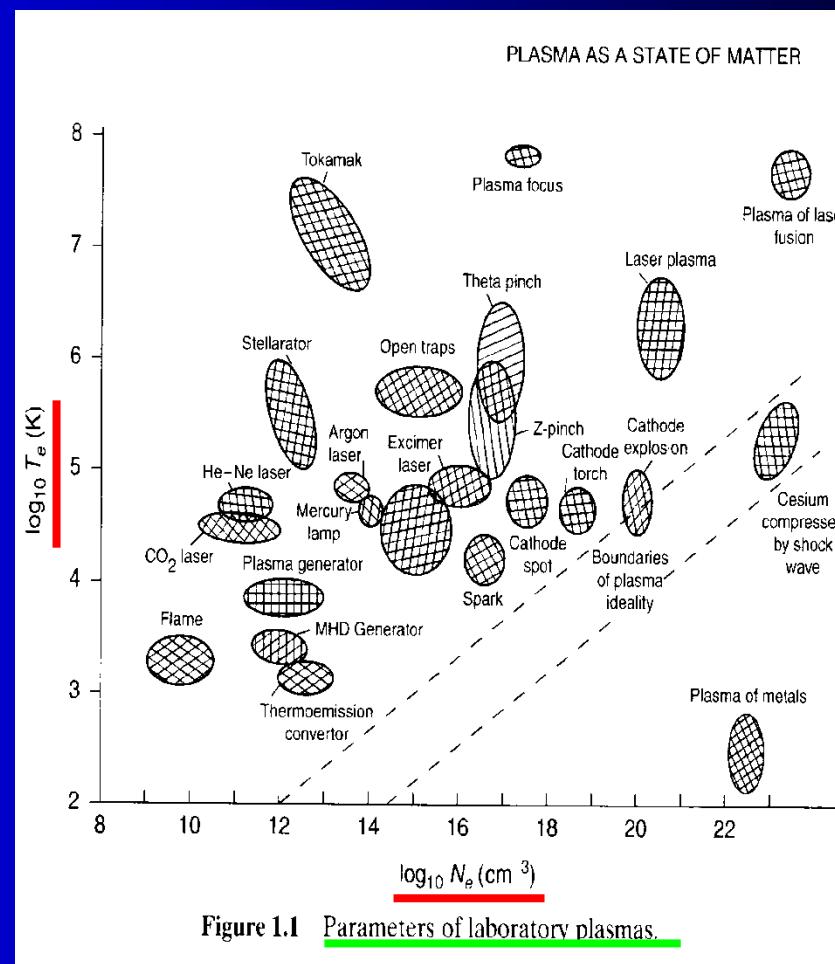
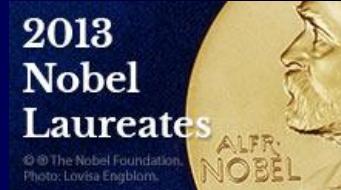
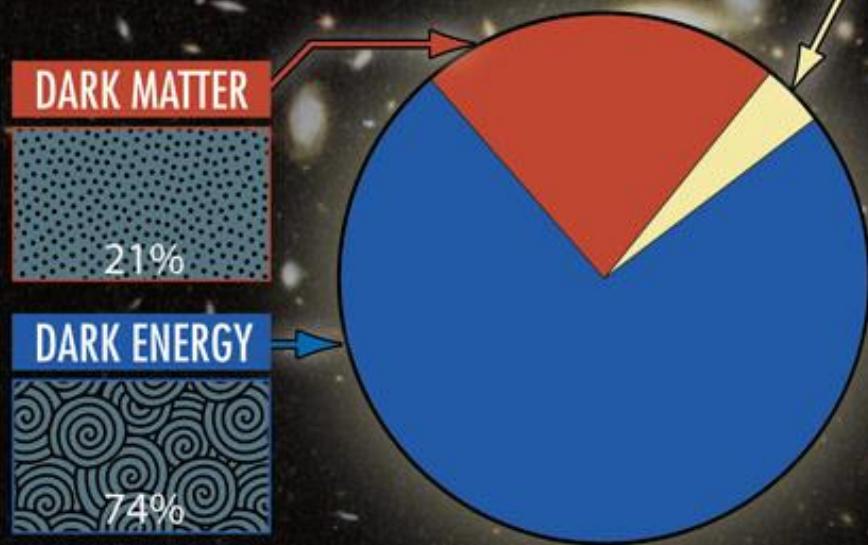


Figure 1.1 Parameters of laboratory plasmas.

## Approximation ....



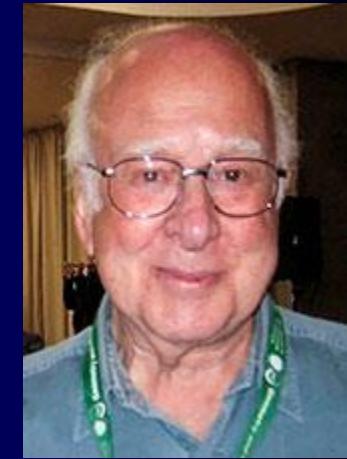
### What The Universe Is Made Of



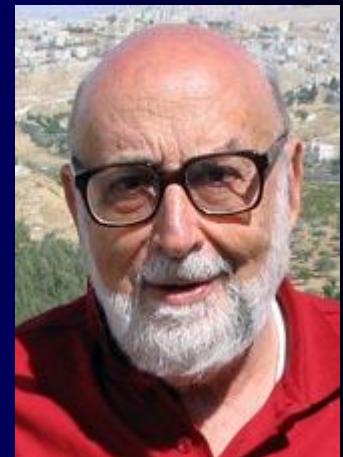
### NORMAL MATTER



Peter W. Higgs



François Englert



### The Nobel Prize in Physics 2013

**François Englert** and **Peter W. Higgs** “for the theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles, and which recently was confirmed through the discovery of the predicted fundamental particle, by the ATLAS and CMS experiments at CERN’s Large Hadron Collider”

**Normal matter ....4.83%**

**... and now it is clear ....**

**Scio me nihil scire**

# Motivation:

e<sup>-</sup>, H<sup>+</sup>, H, H<sup>-</sup>, H<sub>2</sub><sup>+</sup>, H<sub>2</sub>, ....H<sub>3</sub><sup>+</sup>

Just for pleasure.

$$\psi(x) \propto \sum_n A_n e^{ip_n x/\hbar},$$

The Orion molecular clouds

© Royal Observatory, Edinburgh/Anglo-Australian Observatory

92.1% of nucleons in the universe are protons  
7.8% are helium nuclei !

H

He

C N O Ne  
Mg Si S Ar  
Fe

The Privilege of Being a Physicist

Victor F. Weisskopf

There are certain obvious privileges that a physicist enjoys in our society. He is reasonably paid; he is given instruments, laboratories, complicated and expensive machines, and he is asked not to make money with these tools, like most other people, but to spend money. Furthermore, he is supposed to do what he himself finds most interesting, and he accounts for what he spends to the money givers in the form of progress reports and scientific papers that are much too specialized to be understood or evaluated by those who give the money—the federal authorities and, in the last analysis, the taxpayer. Still, we believe that the pursuit of science by the [redacted] ported by the p have to look dee ence to society a physics only; we ral sciences, bu ences, that is, formed without



*Cosmic Abundance  
of some elements*

Element	Abundance
hydrogen (H)	1.000.000
helium	80.147
oxygen	739
carbon	445
neon	138
nitrogen	91
magnesium	40
Silicon	37
Sulfur	19

"Intelligent play with simple, natural phenomena, the joys of discovery of unexpected experiences, are much better ways of learning to think than any teaching by rote."

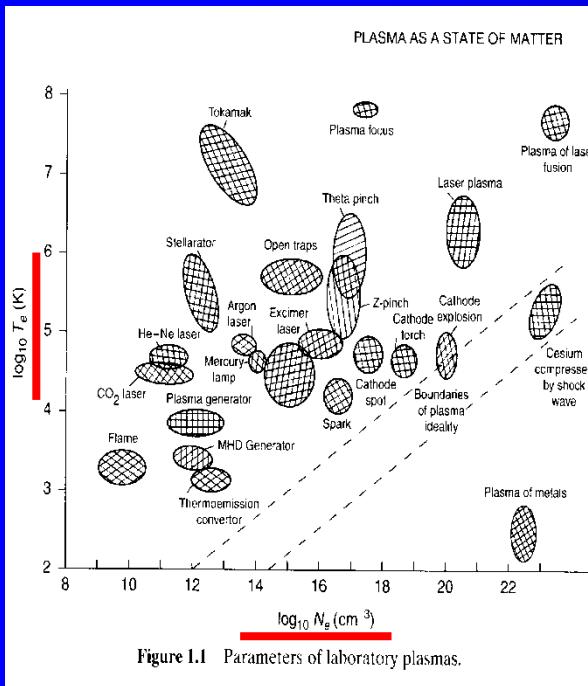
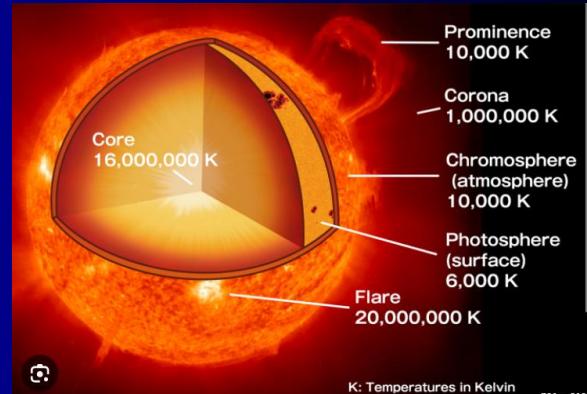
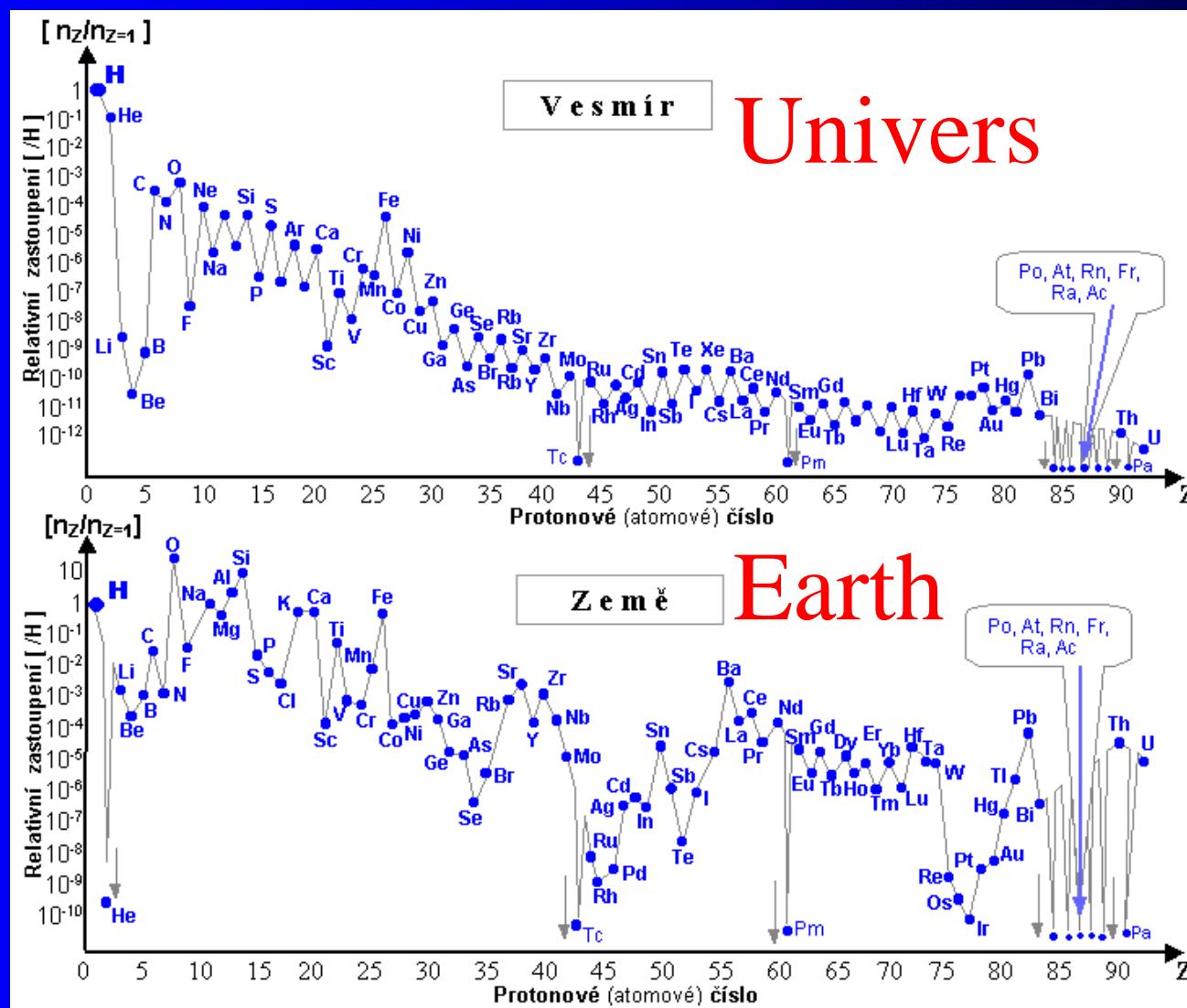


Figure 1.1 Parameters of laboratory plasmas.



### Typical ranges of plasma parameters

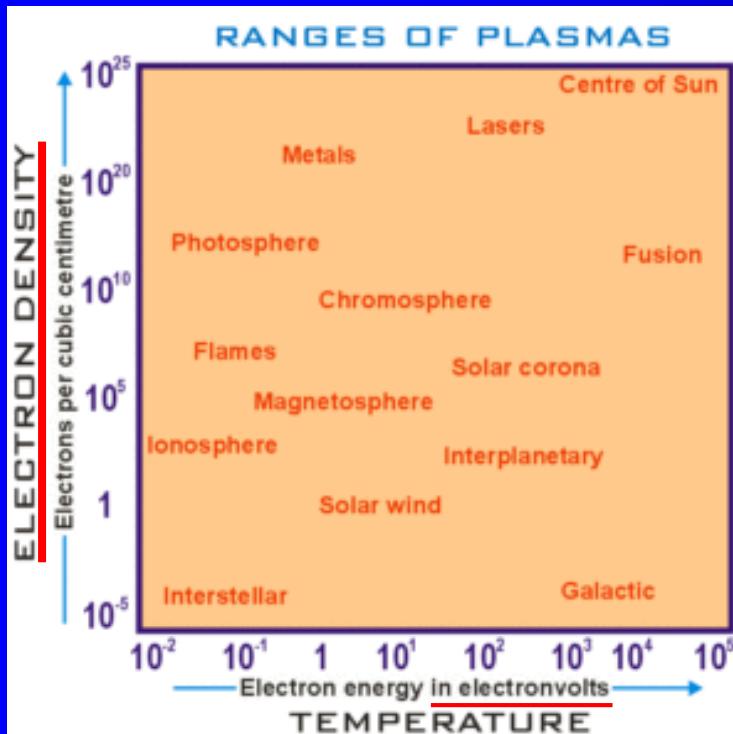
Characteristic	Terrestrial plasmas	Cosmic plasmas
<b>Size</b> in metres	$10^{-6}$ m (lab plasmas) to $10^2$ m (lightning)	$10^{-6}$ m (spacecraft sheath) to $10^{25}$ m (intergalactic nebula)
<b>Lifetime</b> in seconds	$10^{-12}$ s (laser-produced plasma) to $10^7$ s (fluorescent lights)	$10^1$ s (solar flares) to $10^{17}$ s (intergalactic plasma)
<b>Density</b> in particles per cubic metre	$10^7$ m <sup>-3</sup> to $10^{32}$ m <sup>-3</sup> (inertial confinement plasma)	$10^0$ (i.e., 1) m <sup>-3</sup> (intergalactic medium) to $10^{30}$ m <sup>-3</sup> (stellar core)
<b>Temperature</b> in kelvins	$\sim 0$ K (crystalline non-neutral plasma) to $10^8$ K (magnetic fusion plasma)	$10^2$ K (aurora) to $10^7$ K (solar core)
<b>Magnetic fields</b> in teslas	$10^{-4}$ T (lab plasma) to $10^3$ T (pulsed-power plasma)	$10^{-12}$ T (intergalactic medium) to $10^{11}$ T (near neutron stars)



Relativní zastoupení prvků v přírodě v závislosti na jejich protonovém (atomovém) čísle  $Z$ , vztažené k vodíku  $Z=1$ .

**Nahoře:** Nynější průměrné zastoupení prvků ve vesmíru. **Dole:** Výskyt prvků na Zemi (v zemské kůře) a terestrických planetách.

Vzhledem k velkému rozpětí hodnot je relativní zastoupení prvků (vztažené k vodíku  $Z=1$ ) na svislé ose vyneseno v logaritmickém měřítku; to ale může zvláště na horním grafu opticky zkreslit velký rozdíl v zastoupení vodíku a hélia oproti těžším prvkům..



## Ranges of plasma parameters

Density increases upwards, temperature increases towards the right. The free electrons in a metal may be considered an electron plasma [1] Plasma parameters can take on values varying by many orders of magnitude, but the properties of plasmas with apparently disparate parameters may be very similar (see plasma scaling). The following chart considers only conventional atomic plasmas and not exotic phenomena like quark gluon plasmas:

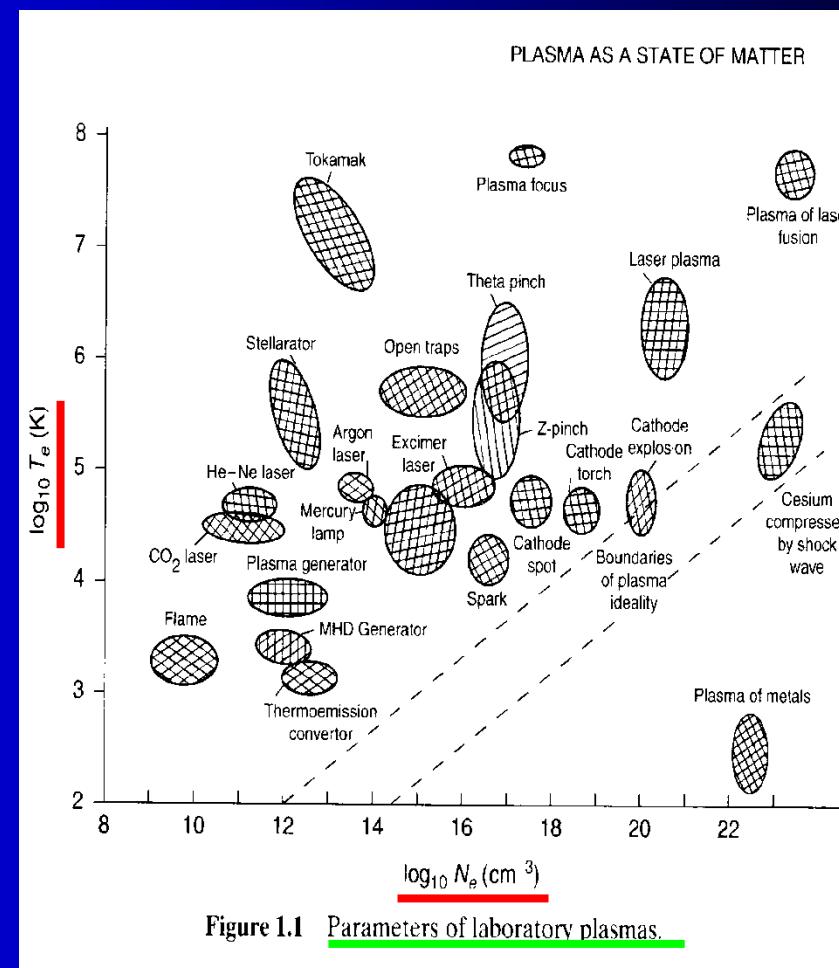


Figure 1.1 Parameters of laboratory plasmas.

05. 10. 2021

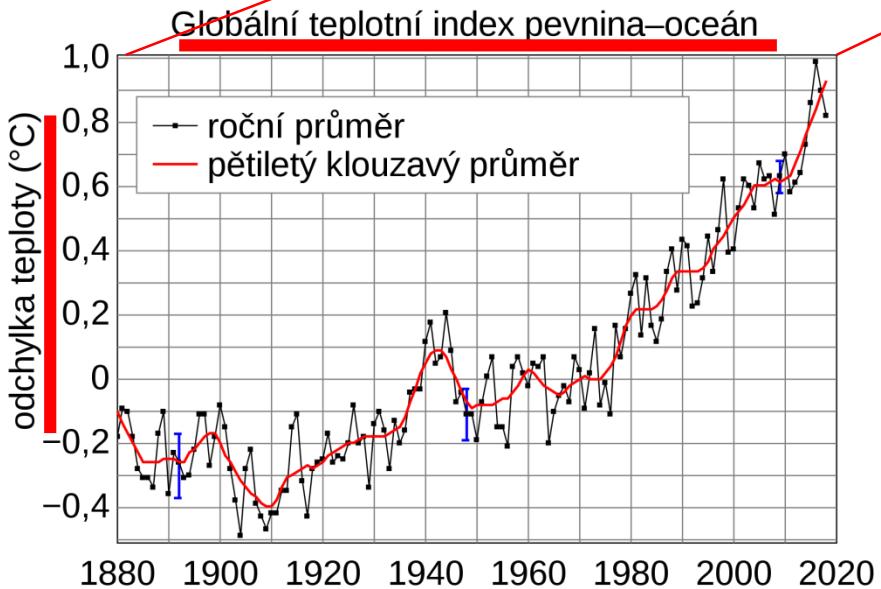
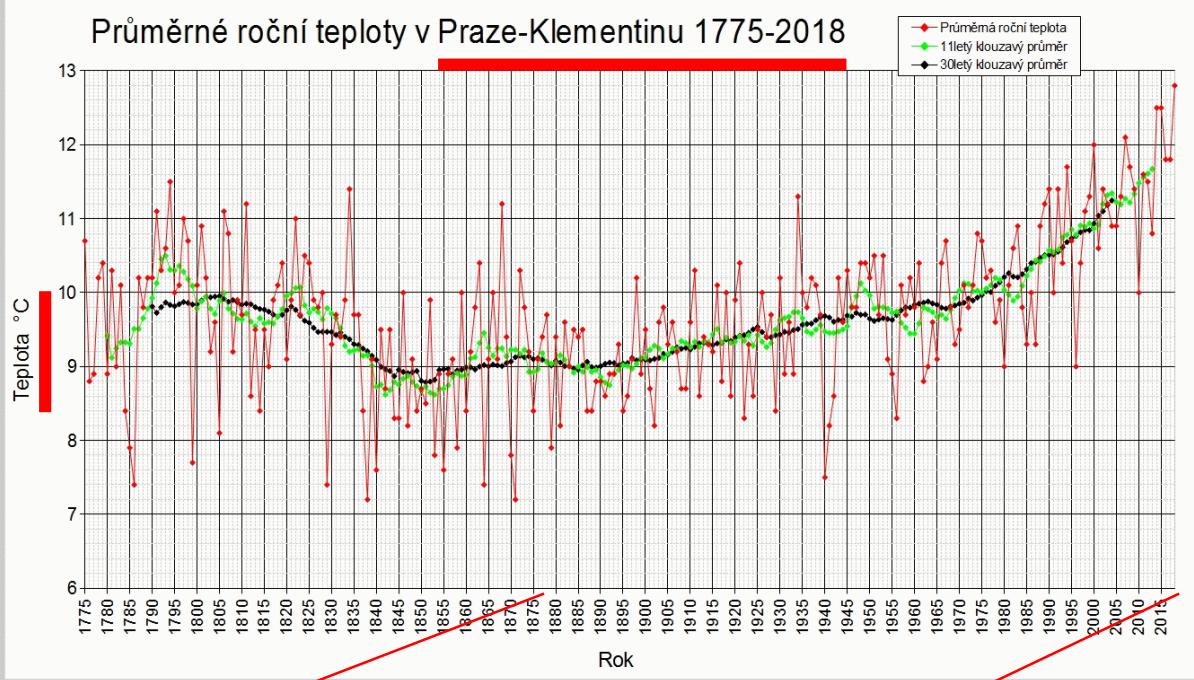
04. 10. 2022

26. 10. 2023



# Information

Průměrné roční teploty v Praze-Klementinu 1775-2018



“Kdo z vás je bez hříchu, první hod’ na ni kamenem”

(see ref.: Nový zákon, ... Ježíš ... hora Olivetska ...)

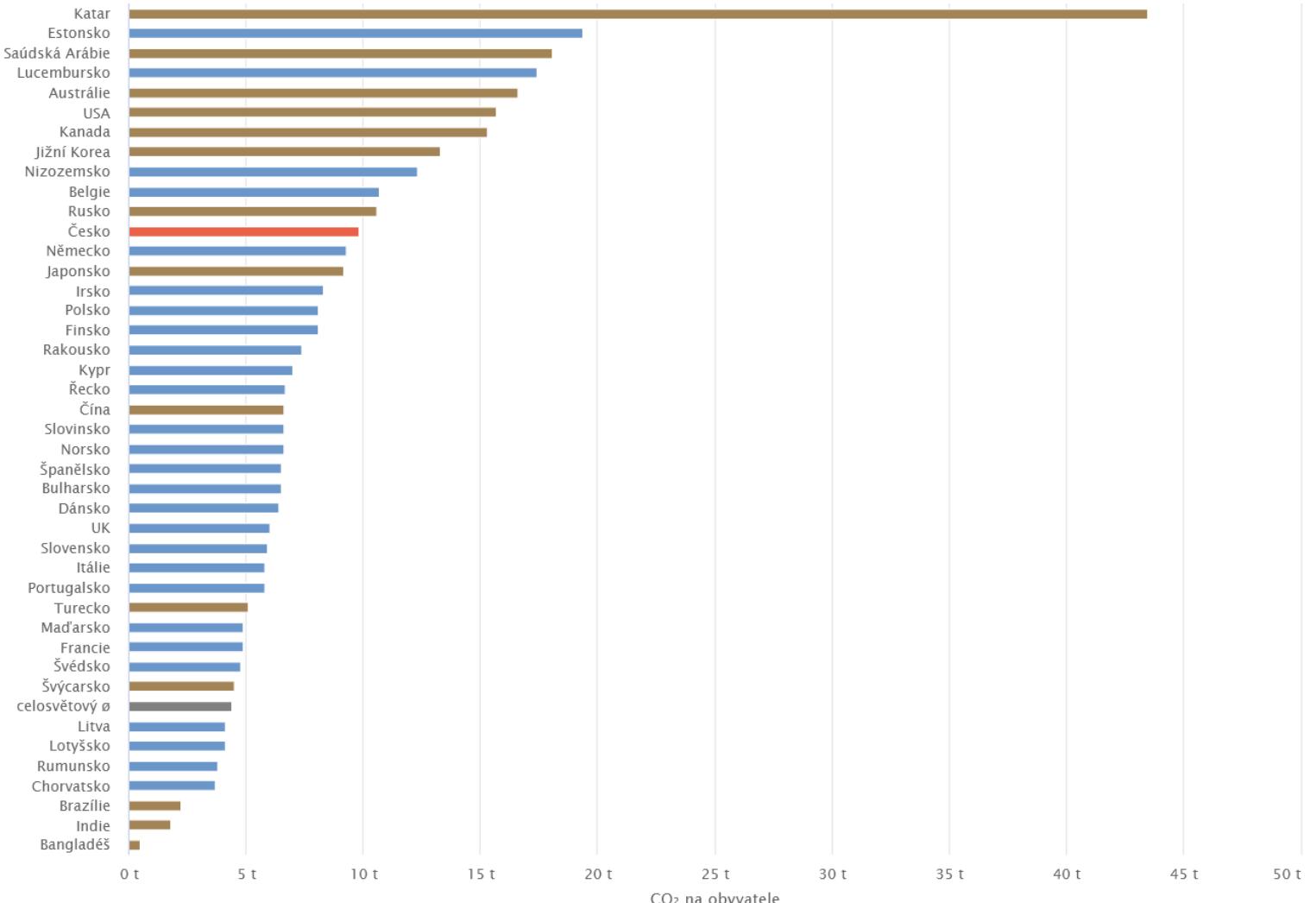
Jesus

*He that is without sin among you, let him be the first to cast a stone at her.*



## Emise CO<sub>2</sub> na hlavu

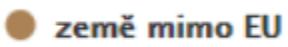
vybrané země, 2017



Česko



země EU



země mimo EU



globální průměr

“Kdo z vás je bez hříchu, první hod' na ni kamenem”

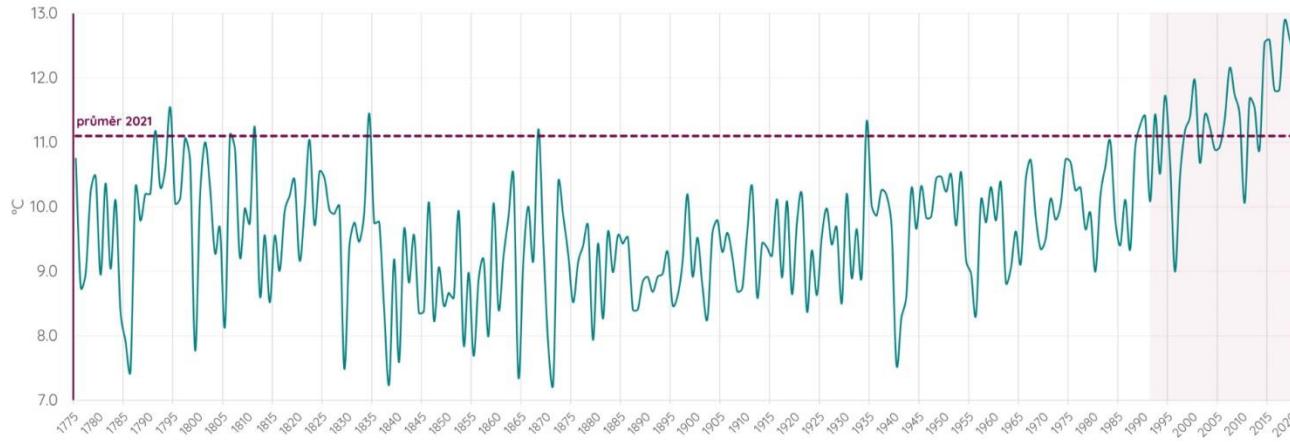
(see ref.: Nový zákon, Jan 8 ... hora Olivetska ...)

Jesus

*He that is without sin among you, let him be the first to cast a stone at her.*



## Průměrná roční teplota 1775–2021, Praha-Klementinum



Graf výše ukazuje průměrné roční teploty na stanici Praha-Klementinum za období 1775 až 2020. V grafu je vyznačena přerušovanou čarou hladina průměrné roční teploty za rok 2021 a vyšrafováno je období 1991 až 2020.

Jak ukažuje výše uvedená infografika, v kontextu posledních 30 let (období 1991 až 2020) a zejména pak poslední dekády (2011 až 2020) opravdu byl rok 2021 chladnější. **Při hodnocení klimatu však nejsou podstatné krátkodobé výkyvy, ale dlouhodobý trend.** Z grafu výše je jasné patrné, že v dlouhodobém hledisku byl i rok 2021 velmi teplý a do roku 1990 bychom za více než 200 let nášly jen 9 roků, které byly v průměru teplejší. Oproti předchozímu třicetiletí 1961-1990 to byl rovněž rok silně nadnormální (+1,1 °C). Trend je zcela zřejmý, a to **dlouhodobé zvyšování teploty**, které se v posledních letech velmi akcelerovalo. To však neznamená, že se nemůže vyskytnout chladnější rok (a stejně tak globální oteplování neznamená, že se v zimě nemohou vyskytnout velmi chladné dny, dlouhodobě jich ale ubívají). Ještě lepším příkladem než rok 2021 je v tomto směru rok 1996 a 2010. Ani tyto dva roky ale nelze považovat za velmi chladné z dlouhodobého hlediska. Při pohledu na celkový průběh je patrné, že rok 1996 byl blízko průměru 1775-1990 a rok 2010 byl z dlouhodobého pohledu teplotně nadprůměrný.

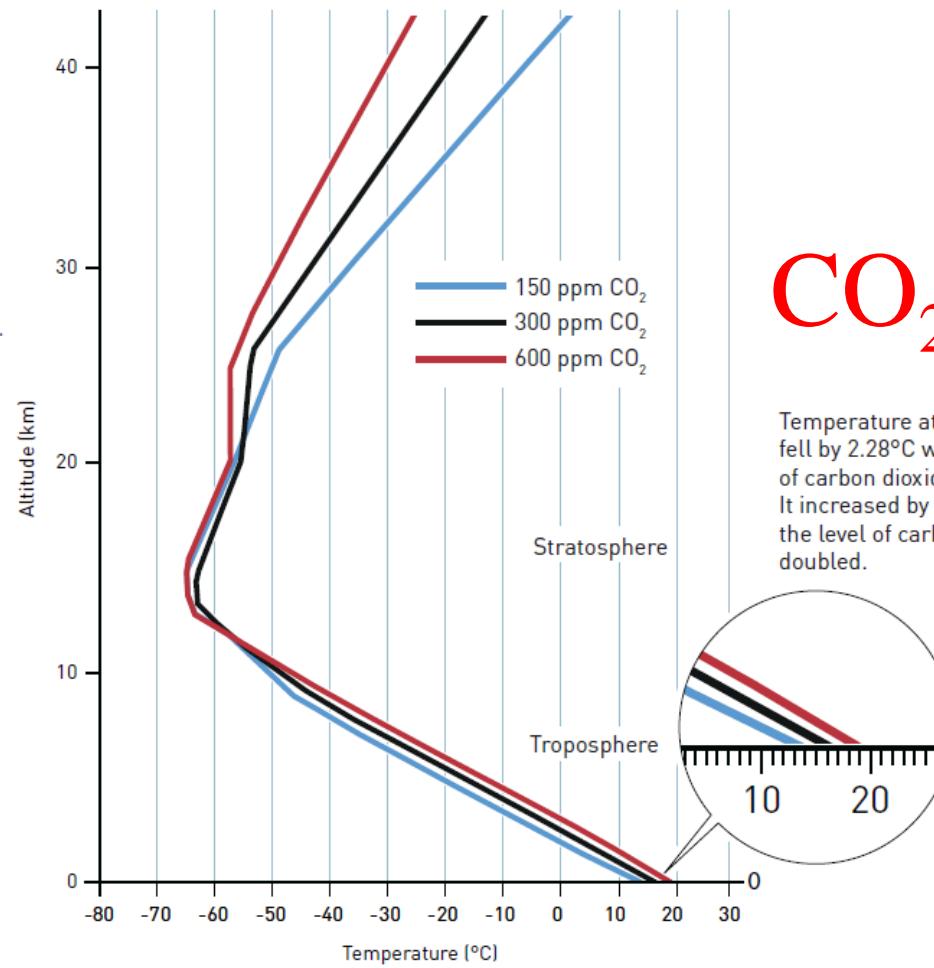
Jáchym Brzina © 2022 @jachym | www.infoviz.cz

Zdroj: Český hydrometeorologický ústav



## Carbon dioxide heats the atmosphere

Increased levels of carbon dioxide lead to higher temperatures in the lower atmosphere, while the upper atmosphere gets colder. Manabe thus confirmed that the variation in temperature is due to increased levels of carbon dioxide; if it was caused by increased solar radiation, the entire atmosphere should have warmed up.

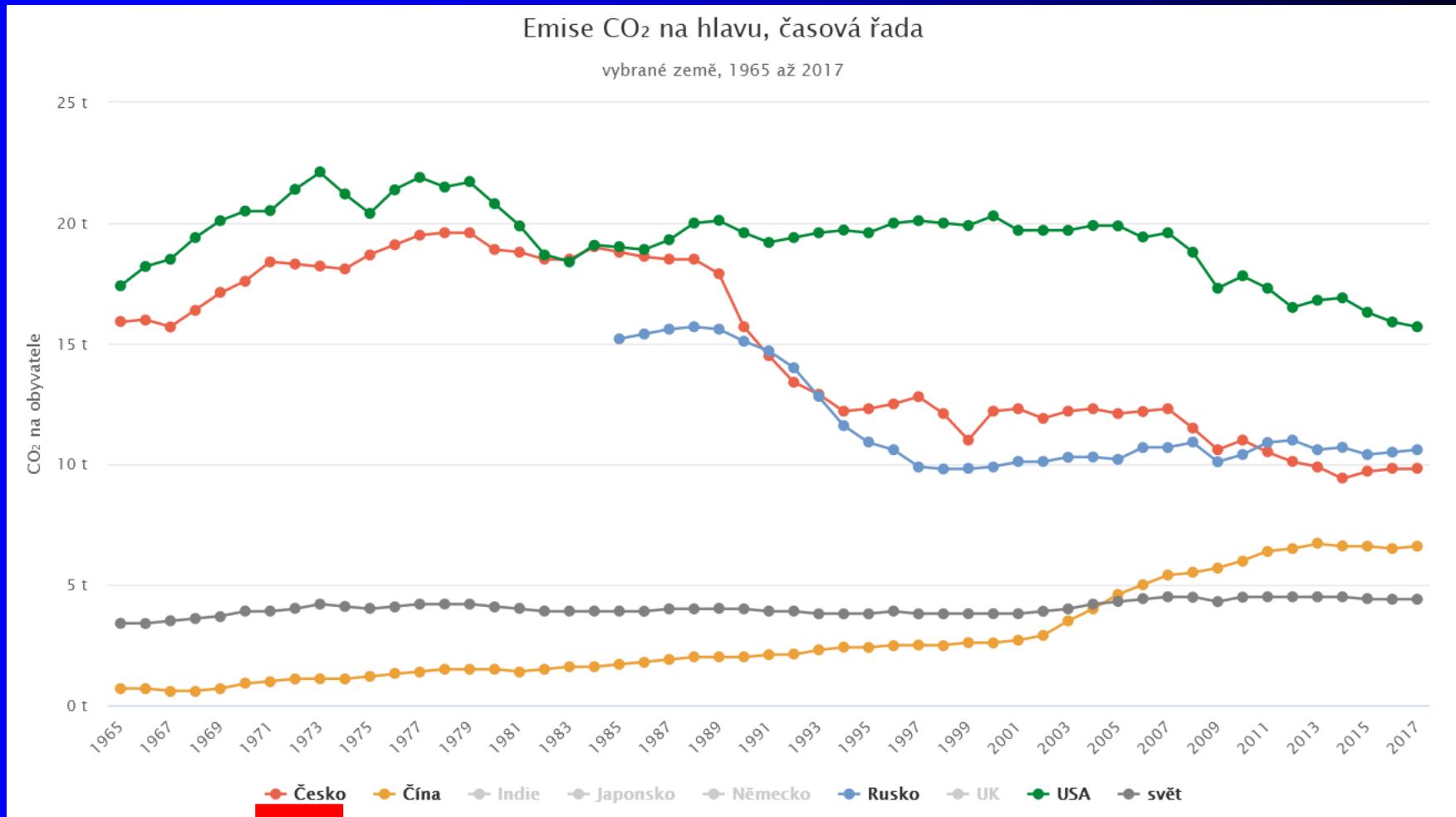


# CO<sub>2</sub>

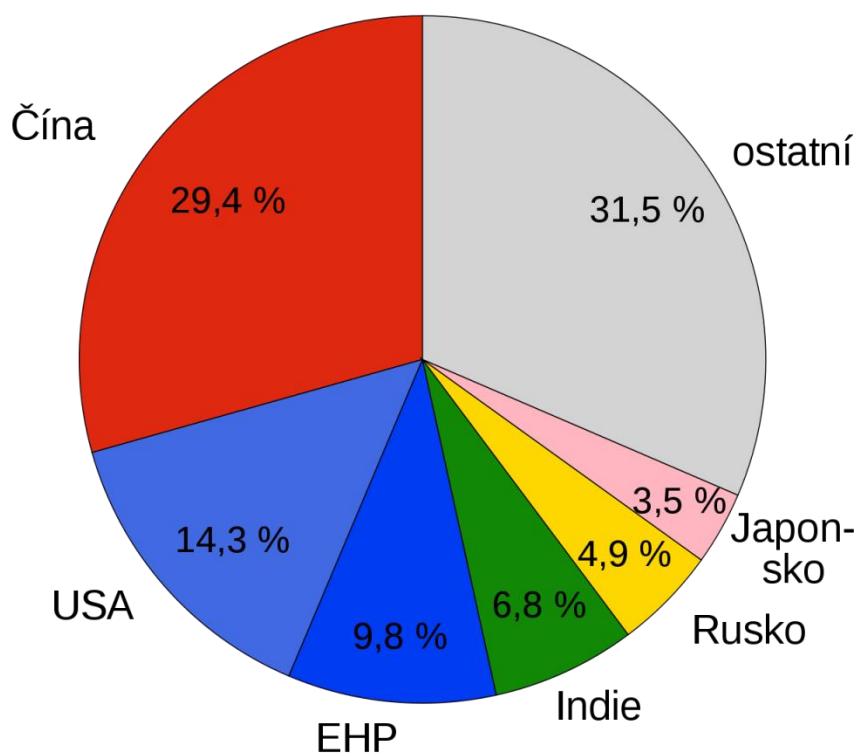
Temperature at the surface fell by 2.28°C when the level of carbon dioxide halved. It increased by 2.36°C when the level of carbon dioxide doubled.

Source: Manabe and Wetherald (1967) Thermal equilibrium of the atmosphere with a given distribution of relative humidity, *Journal of the atmospheric sciences*, Vol. 24, Nr 3, May.

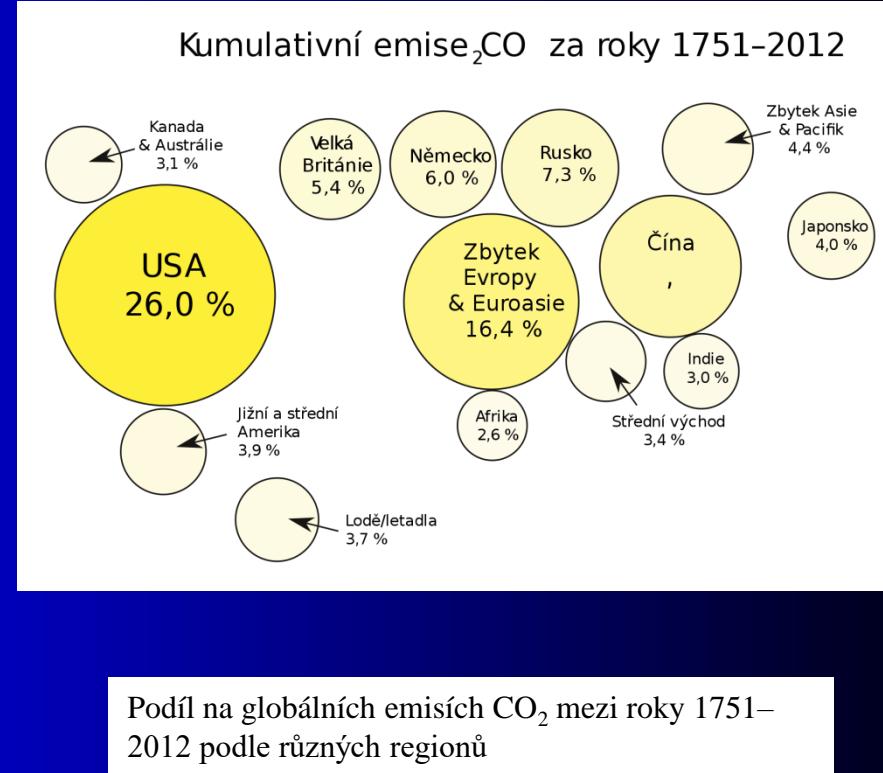
# Emissions of CO<sub>2</sub> per person



## Not actualized, approximation



Největší producenti CO<sub>2</sub> na světě

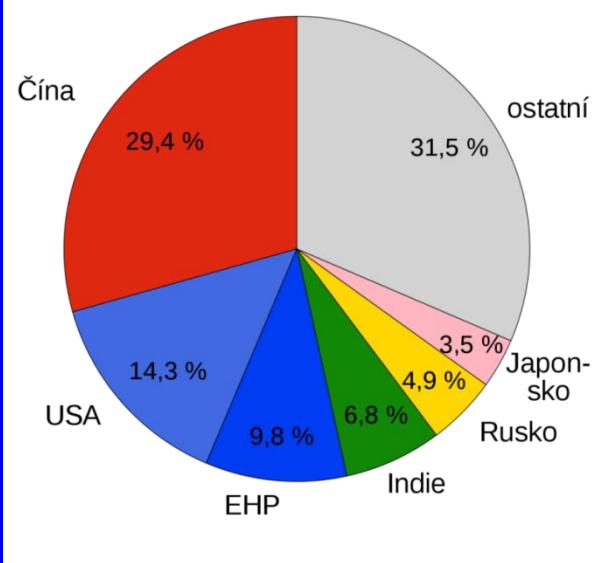


Kdo z vás je bez hříchu, první hod' na ni kamenem

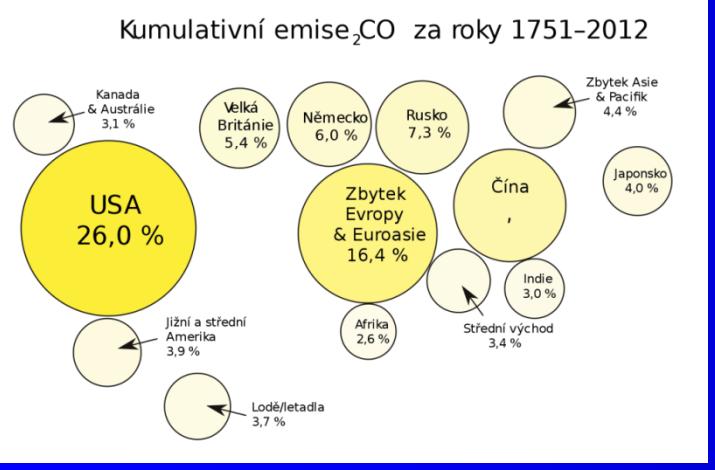
Jesus

*He that is without sin among you, let him be the first to cast a stone at her.*

## Not actualized, approximation



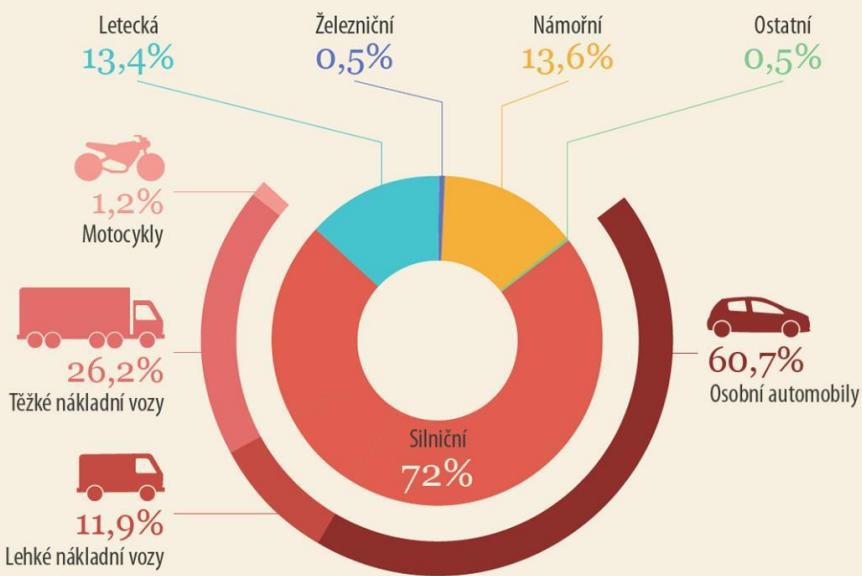
Největší producenti CO<sub>2</sub> na světě



Podíl na globálních emisích CO<sub>2</sub> mezi roky 1751–2012 podle různých regionů

## EMISE CO<sub>2</sub> PRODUKOVANÉ V DOPRAVĚ

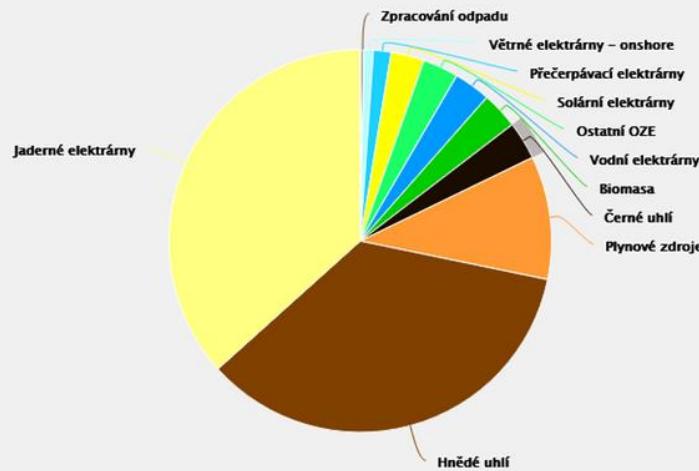
Podíl emisí podle druhu dopravy (2016)



Zdroj: Evropská agentura pro životní prostředí

## Česká republika: Podíl zdrojů na výrobě elektřiny

Data od: 1. 1. 2021 do: 31. 12. 2021

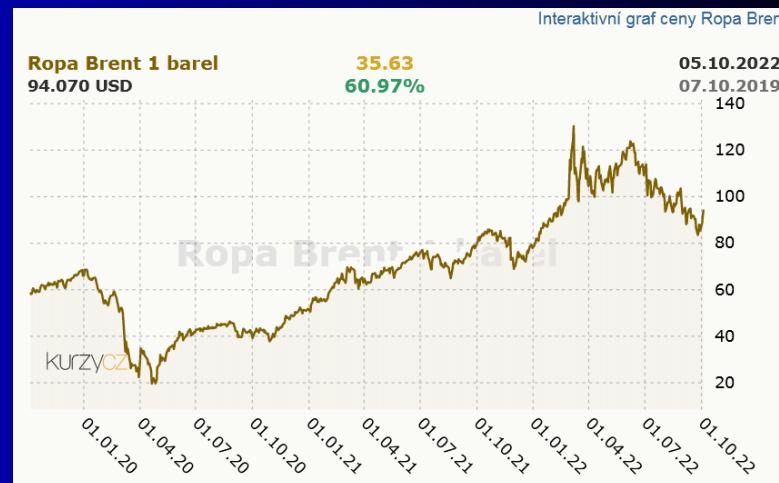


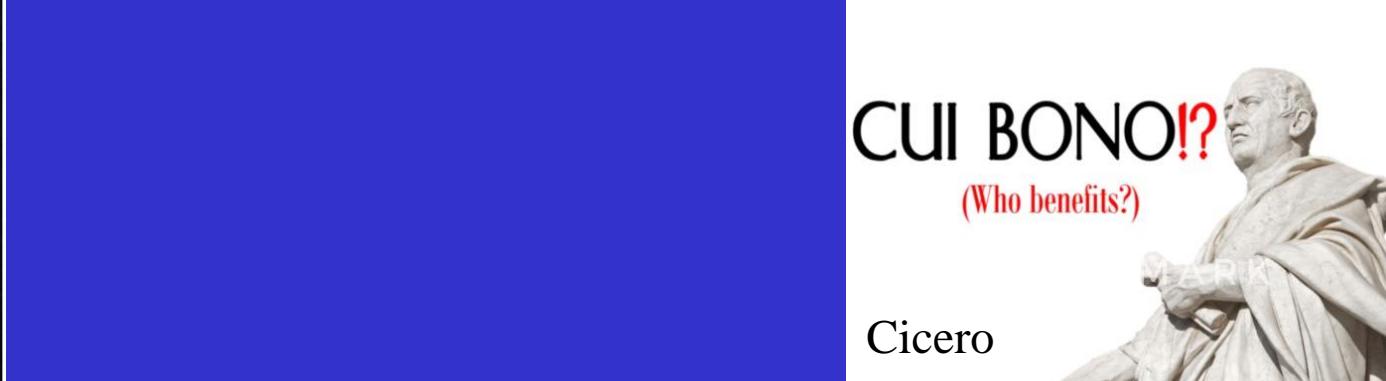
## Podíl zdrojů na výrobě elektřiny v roce 2021 (v %)

	Česko	Slovensko	Maďarsko	Rakousko	Německo	Polsko	Francie
Jaderné elektrárny	36.6	54.3	51.2	0	13	0	70.4
Hnědé uhlí	35.1	3.5	10.3	0	19.5	26.1	0
Plynové zdroje	10.4	13.7	29.2	16.1	10.4	8	6.4
Černé uhlí	3.2	1.3	0	0	10.3	50.4	0.8
Biomasa	3.1	3.1	3.8	2.6	7.8	1.2	0.6
Vodní elektrárny	4.7	15.5	0.6	65.2	4.7	1.8	11.9
Fotovoltaické elektrárny	2.9	2.1	0	1.6	9.4	2.9	2.7
Větrné elektrárny	0.9	0	2.1	12.6	22.8	9.6	6.9
Ostatní obnovitelné zdroje	3	1.8	0.8	1.6	1.5	0	0.3
Ostatní	0.1	4.7	2	0.3	0.6	0	0
<b>Celkem OZE</b>	<b>14.6</b>	<b>22.5</b>	<b>7.3</b>	<b>83.6</b>	<b>46.2</b>	<b>15.5</b>	<b>22.4</b>

Cui bono?  
Qui Bonum

Interaktivní graf ceny Ropa Brent

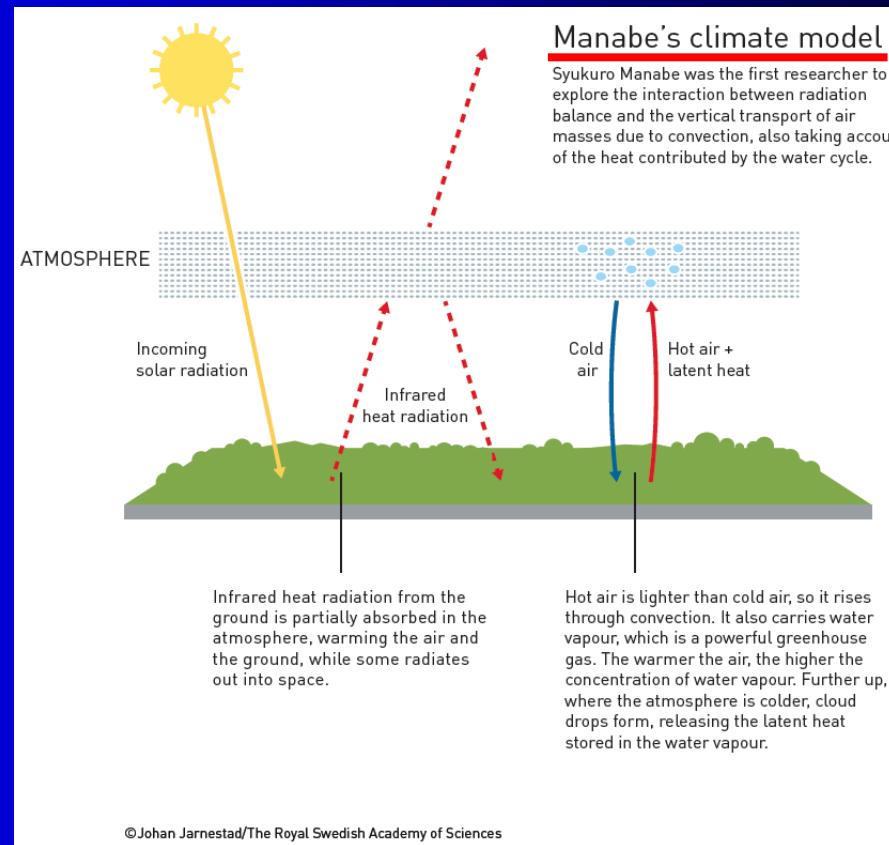




**Manabe's work in the 1960s demonstrated how increased levels of carbon dioxide in the atmosphere caused the Earth's temperature to rise. In doing so, he "laid the foundation for the development of current climate models," the Royal Swedish Academy of Sciences said in a statement.**

A decade later, Hasselmann "created a model that links together weather and climate."

Parisi's discoveries, meanwhile, "make it possible to understand and describe many different and apparently entirely random complex materials and phenomena." This is not only true for physics but also for other areas, such as mathematics, biology, neuroscience and machine learning, the academy added.

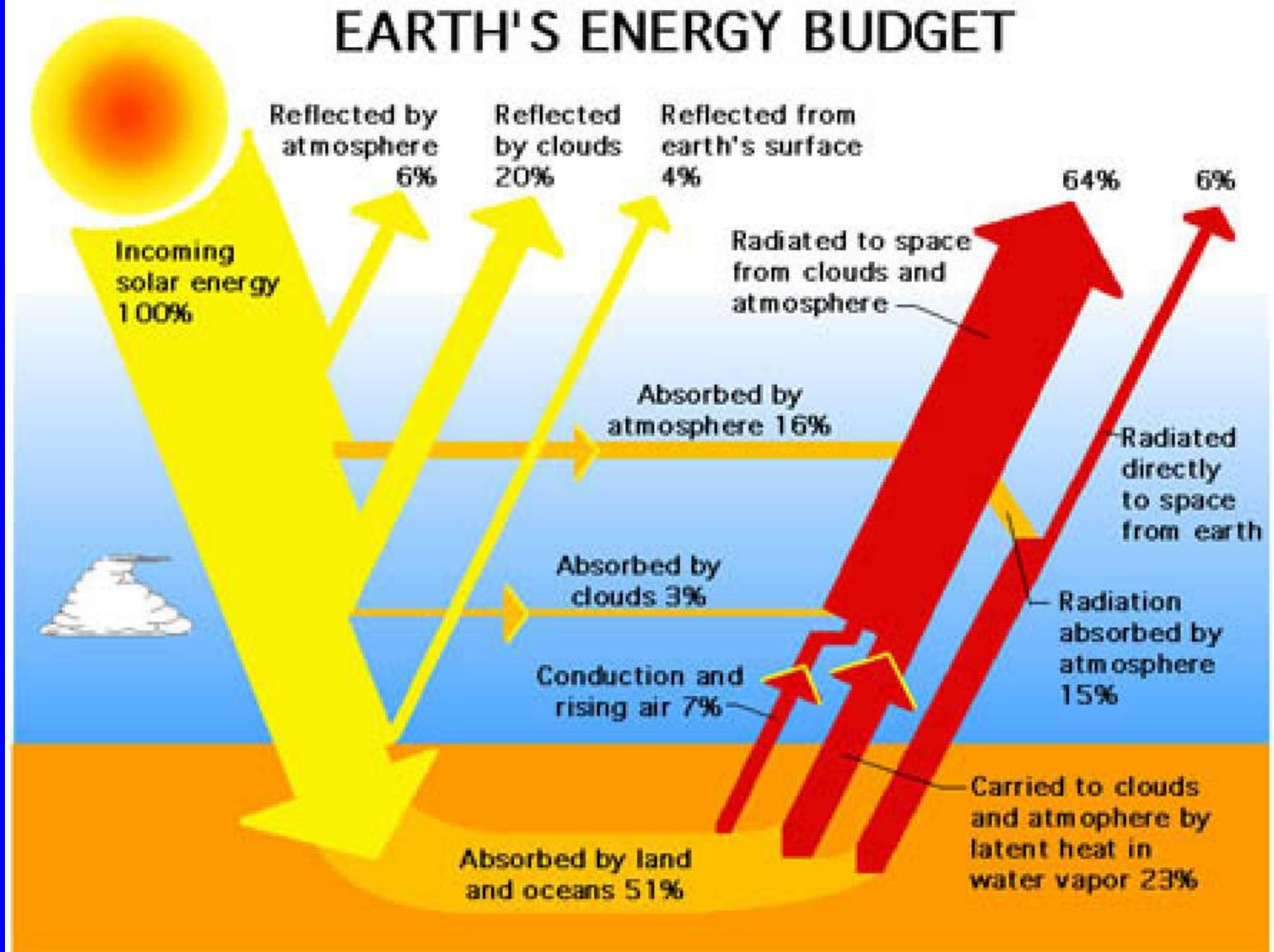


05. 10. 2021



The committee's decision to recognize pioneering work on climate change comes weeks before the world's leaders meet at COP26, a crucial summit in the United Kingdom.

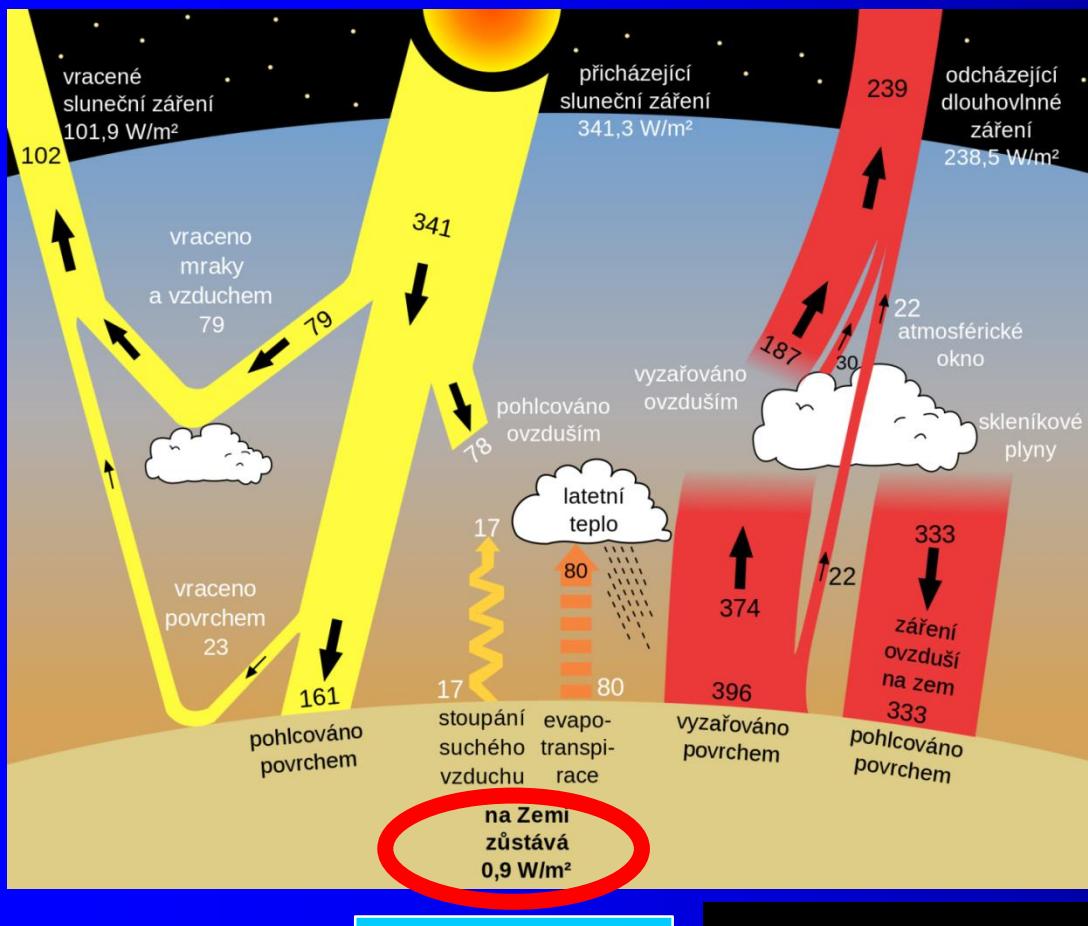
# EARTH'S ENERGY BUDGET



## Not actualized, approximation

wikipedia.org/wiki/Terestriální\_záření

units  $\text{W/m}^2$



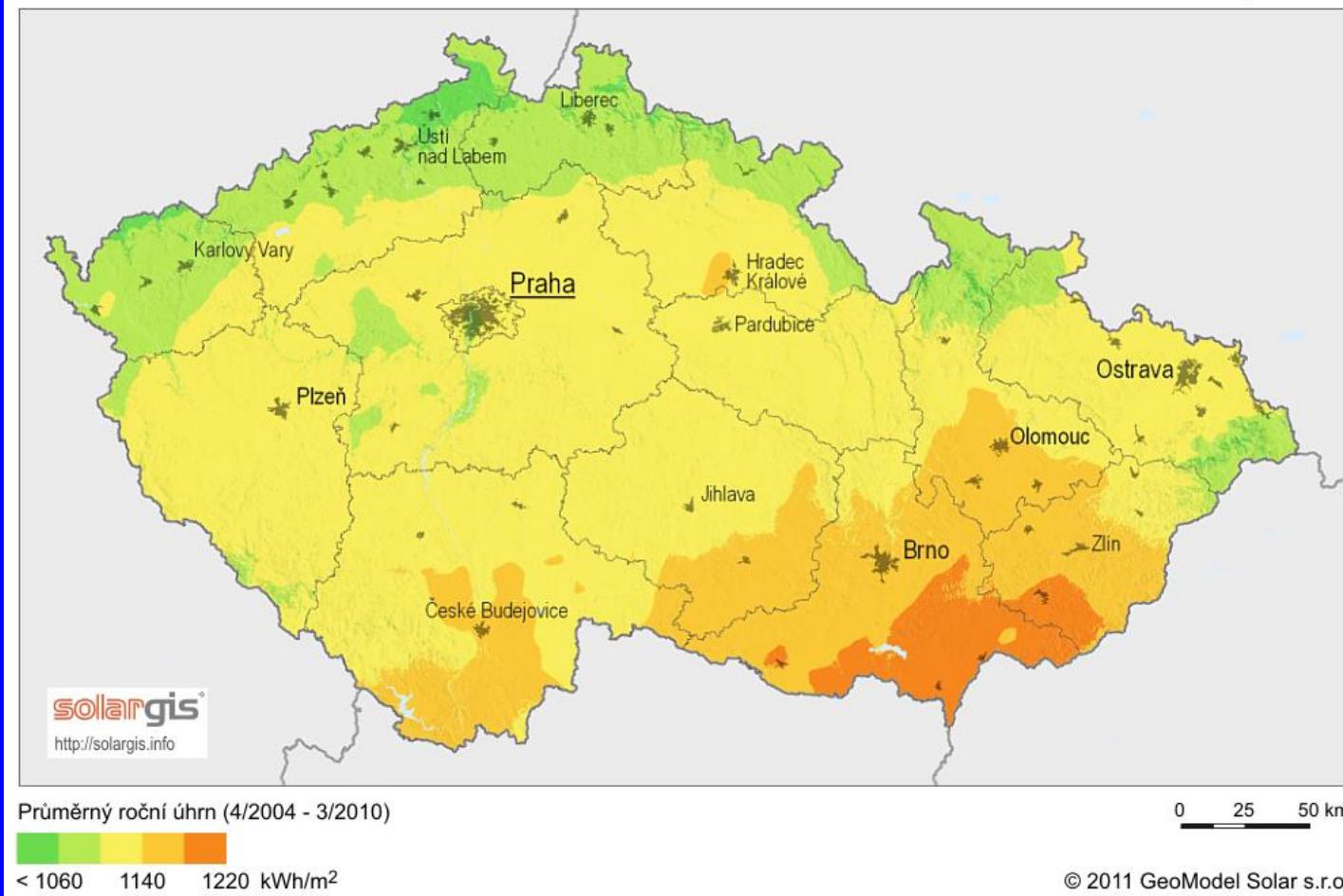
$$\text{difference } (E_{\text{in}} - E_{\text{out}}) = 0.9 \text{ W/m}^2$$

Krátkovlnné záření ze Slunce dopadající na zemský povrch a atmosféru. Dlouhovlnná část záření je emitována z povrchu a téměř zcela absorbována do atmosféry.

V tepelné rovnováze je absorbovaná energie z atmosféry ~ stejná jako ta vydávaná do vesmíru.

Čísla ukazují výkon záření ve wattech na metr čtvereční y období let 2000–2004

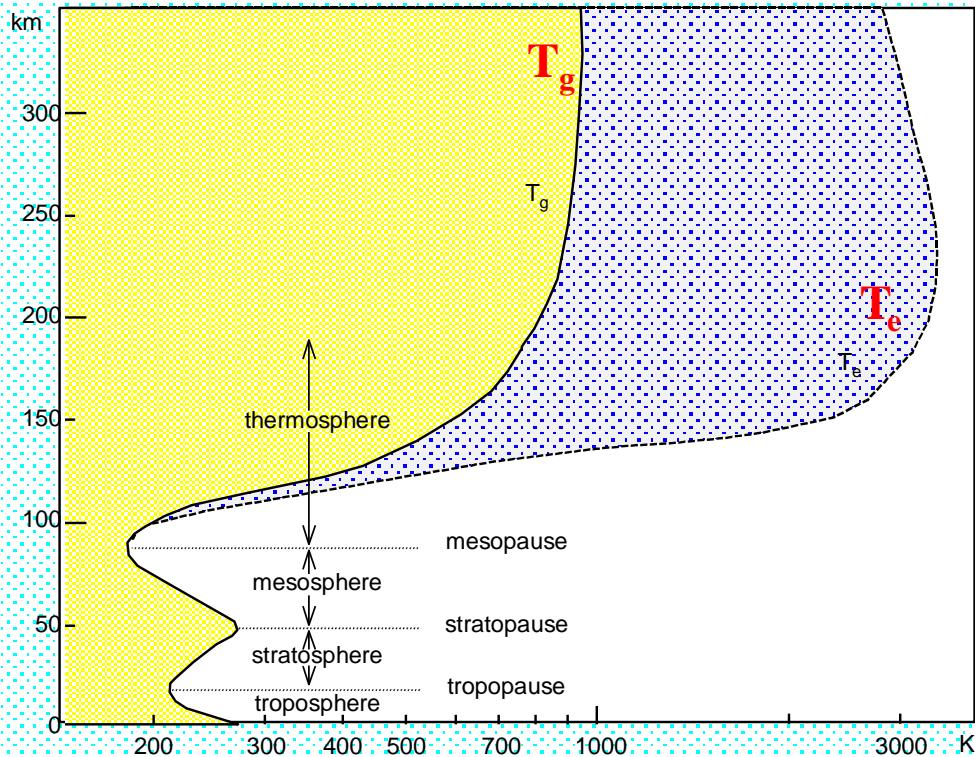
Průměrná hustota toku energie ze zemského povrchu vzhůru činí asi  $400 \text{ W/m}^2$ , což odpovídá teplotě  $16^\circ\text{C}$ ; hustota toku, který Země vyzařuje do vesmíru, činí ale jen asi  $240 \text{ W/m}^2$  a odpovídá to teplotě zhruba  $255 \text{ K}$ . Terestriální (též terestrické, pozemské) záření je v naprosté většině dlouhovlnné infračervené záření.



.... elektřiny stanoven na **6 Kč/kWh s DPH**  
.... plynu na **3 Kč/kWh s DPH**.

# Temperature (???) in the ionosphere

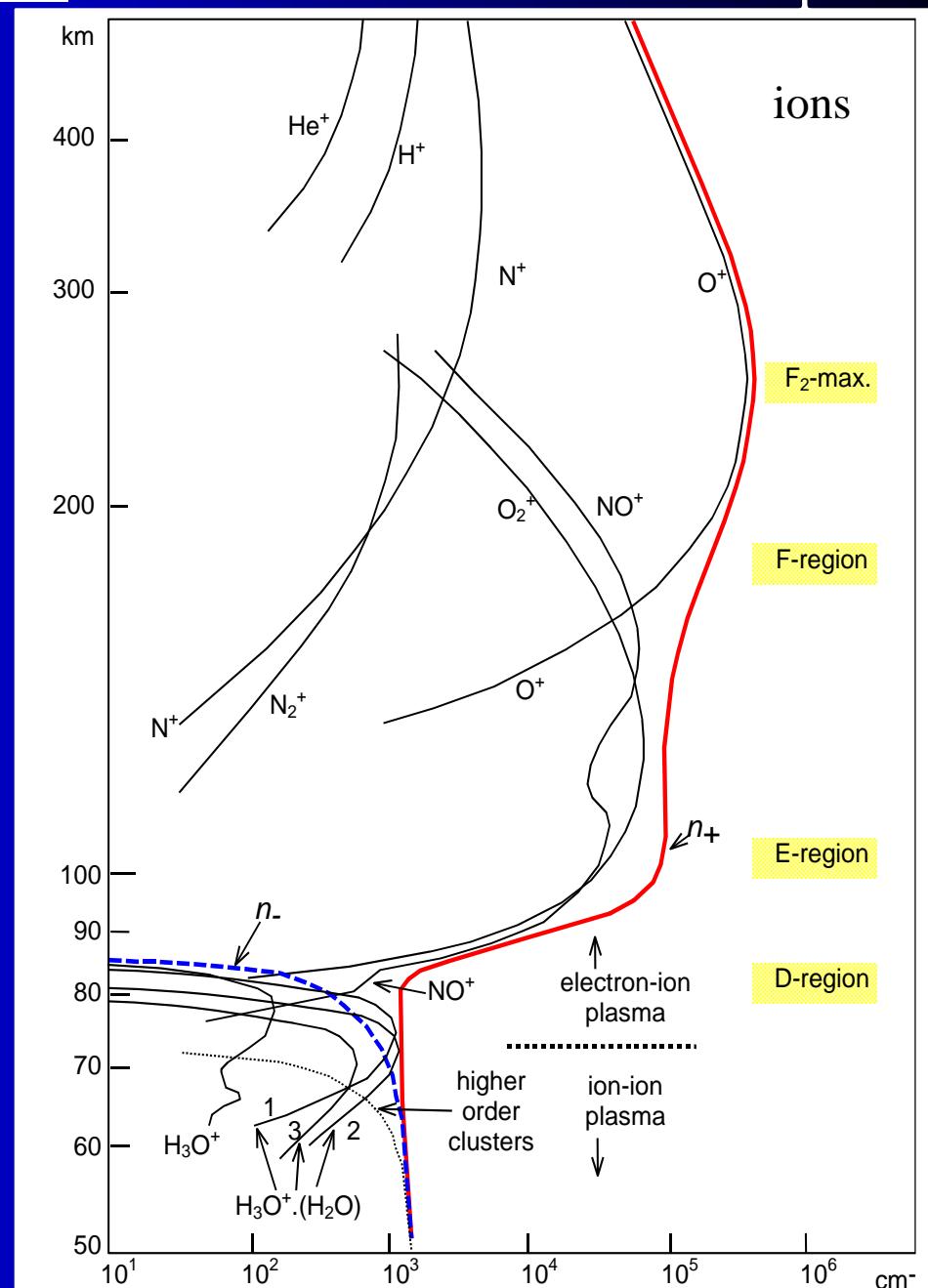
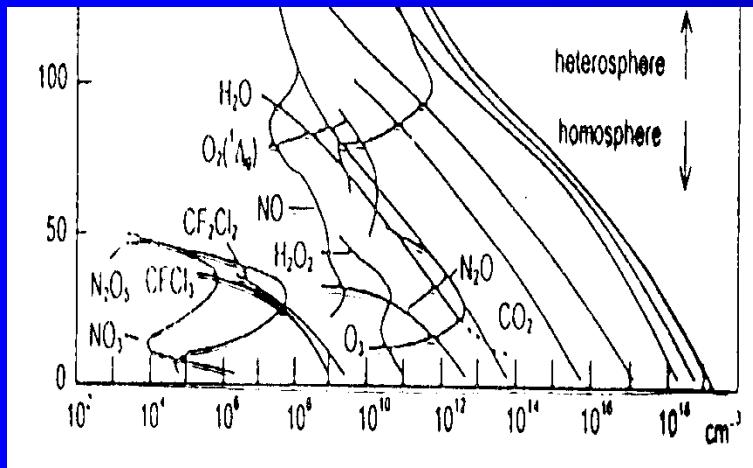
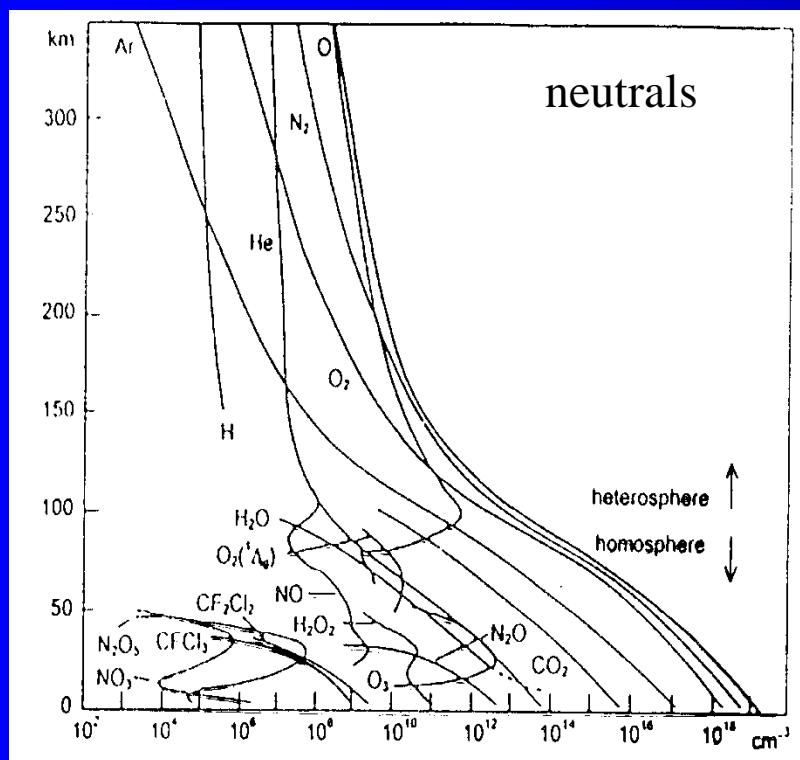
## Temperatures in the ionosphere



# Ions chemistry

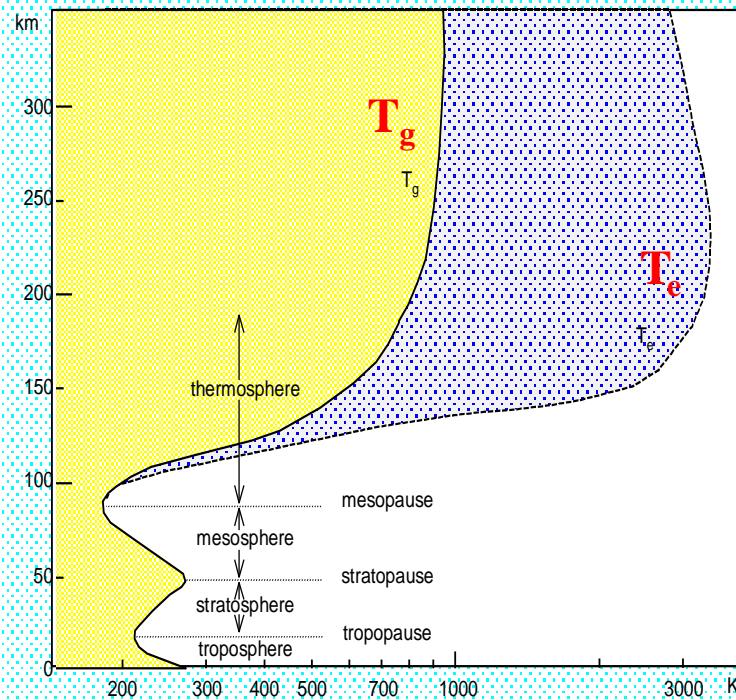
$$n_0 = 2,686\,781\,1(15) \times 10^{19} \text{ cm}^{-3}$$

# Ions in the terrestrial atmosphere

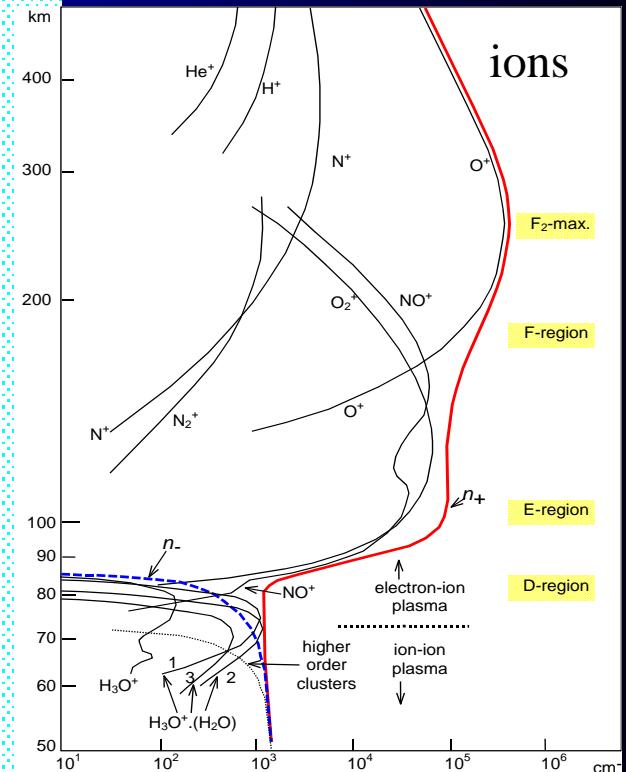


# Ions in the terrestrial atmosphere

## Temperatures in the ionosphere

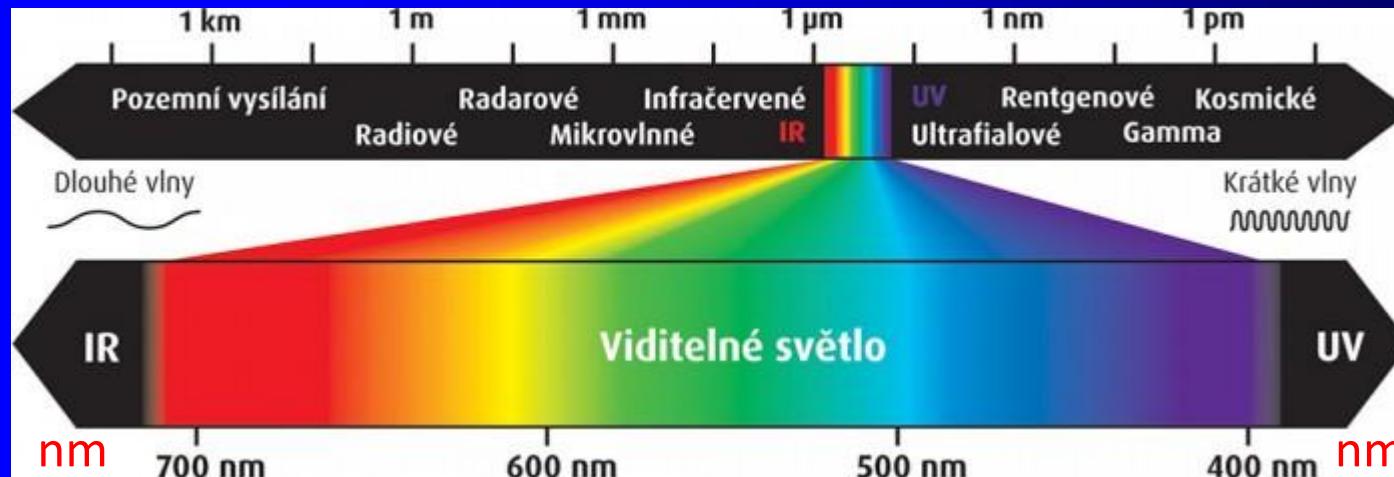


Recombination??  $\alpha(T)$



# Spektrum elektromagnetického záření

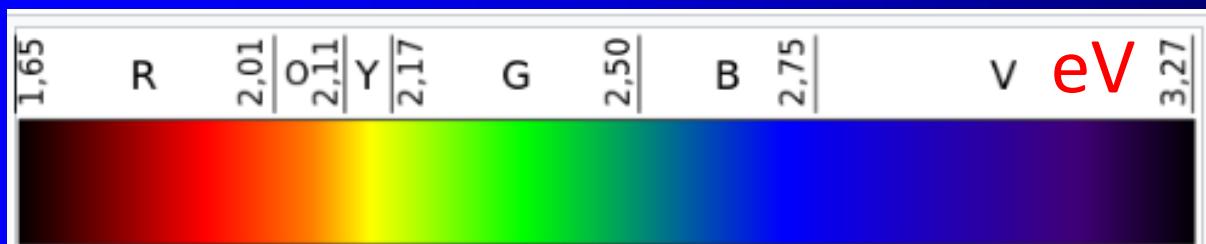
Information



**Viditelné světlo** - elektromagnetické záření v rozmezí vlnových délek 380–760 nm.

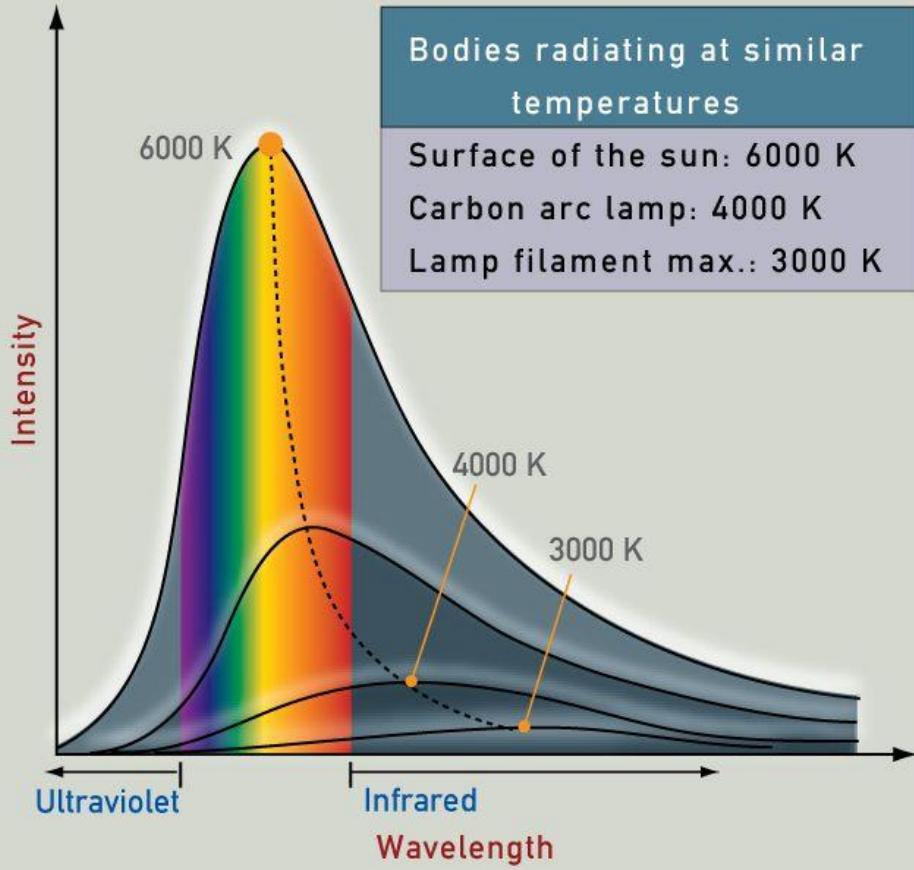
Visible light

eV



Barva světla přímo souvisí s energií fotonu. Lidské oko vnímá rozsah 1,65÷3,27 eV.

# Blackbody Radiation Curves



SURFACE TEMPERATURE OF THE SUN & EARTH



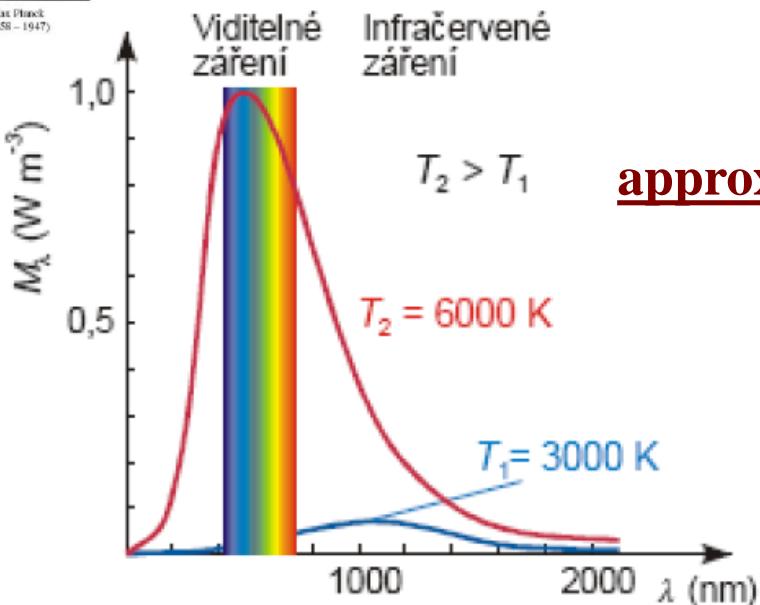
6,000K (5,727°C or 10,340°F)

288K (15°C or 59°F)



Max Planck  
(1858 – 1947)

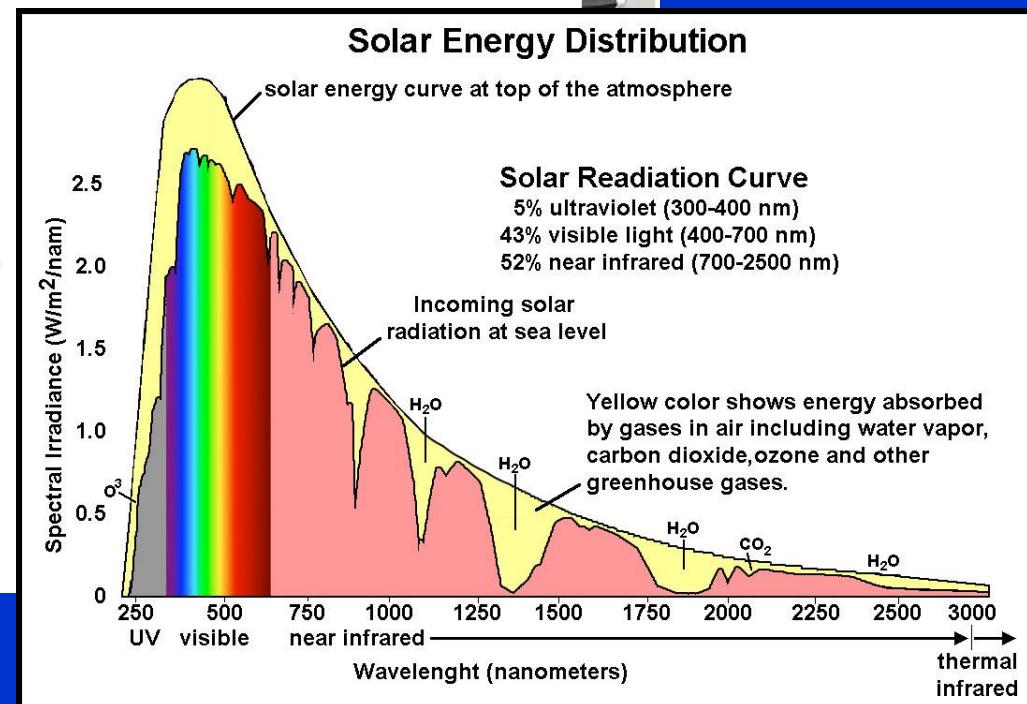
## Záření černého tělesa



approximately

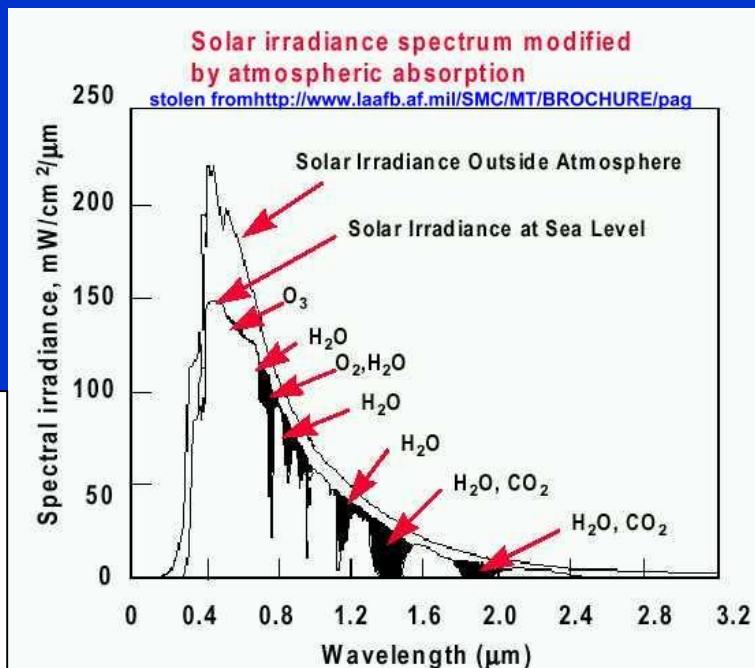
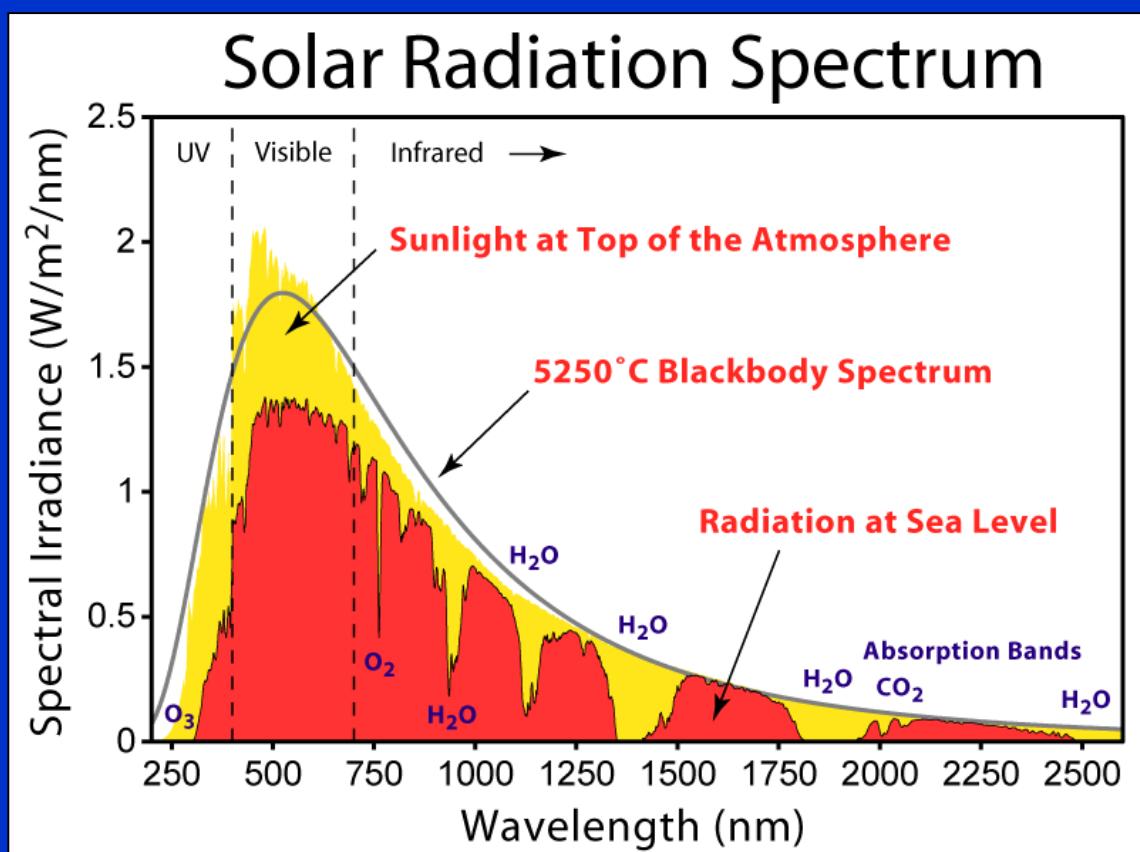


Průběh spektrální intenzity vyzařování v závislosti na vlnové délce a teplotě.  
S rostoucí termodynamickou teplotou tělesa se zvyšuje maximum spektrální intenzity vyzařování a posouvá se směrem k nižší vlnové délce

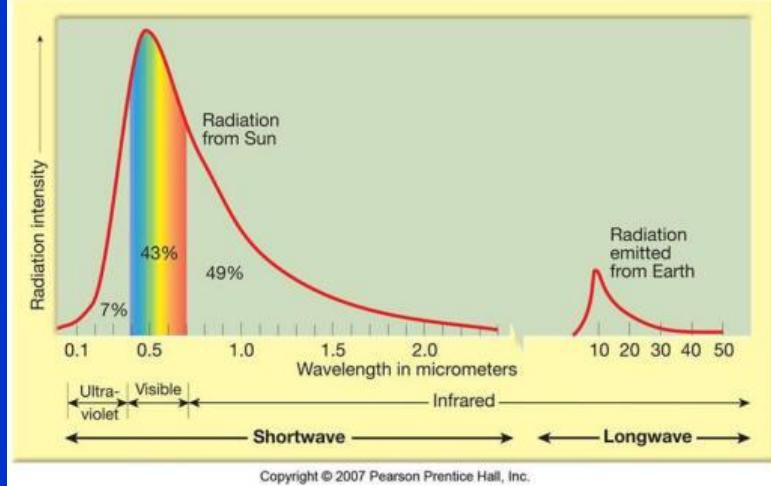


approximately

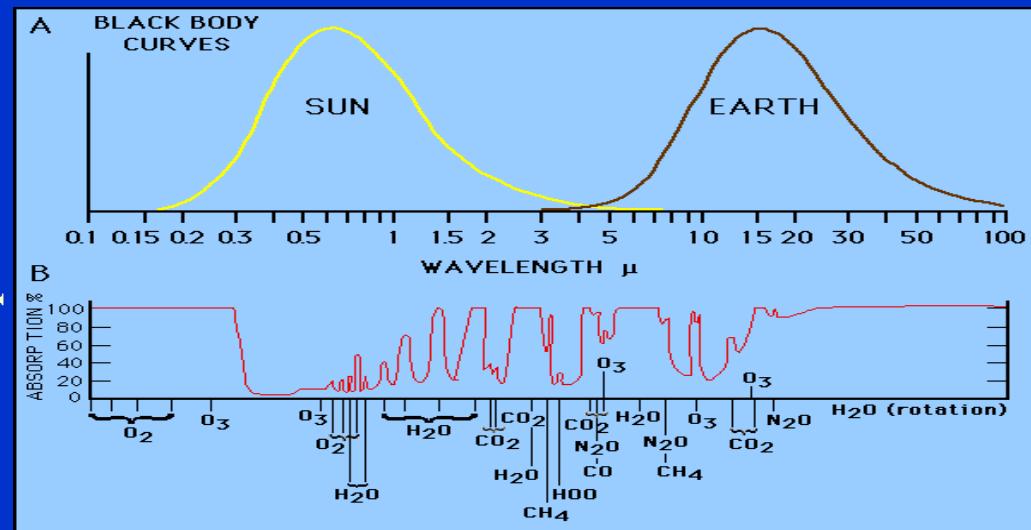
# Spectrum of solar radiation modified by atmospheric absorption



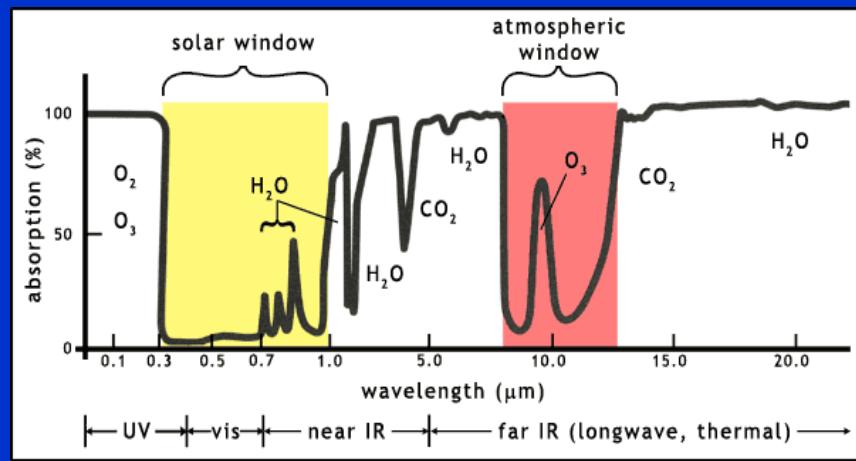
# Detail 0.1-100 $\mu\text{m}$



Absorption %

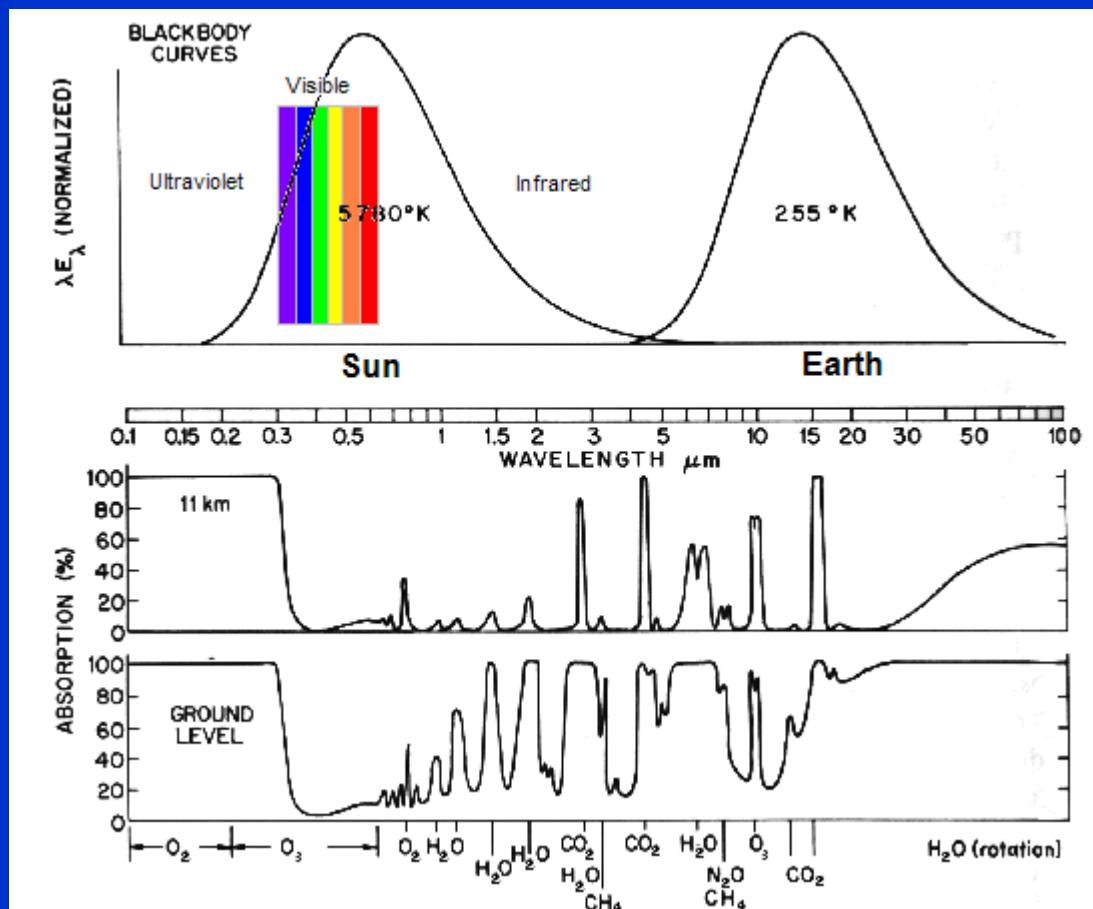
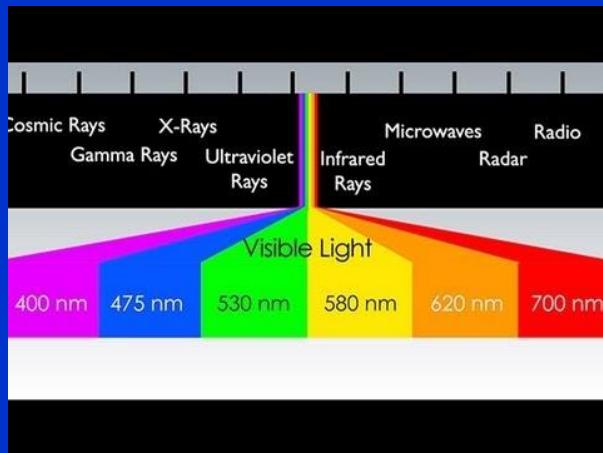


Absorption %



**Figure 3.** The wavelengths of incoming solar radiation and emitted radiation absorbed by the Earth's atmosphere, showing the solar window and atmospheric (thermal) window. The graph shows the regions of the electromagnetic spectrum (light) that are absorbed by specific molecules. Key: CO<sub>2</sub>, carbon dioxide; H<sub>2</sub>O, water; IR, infrared light; O<sub>2</sub>, oxygen; O<sub>3</sub>, ozone; UV, ultraviolet light; vis, visible light (adapted from a figure in Turco 2002, p334)

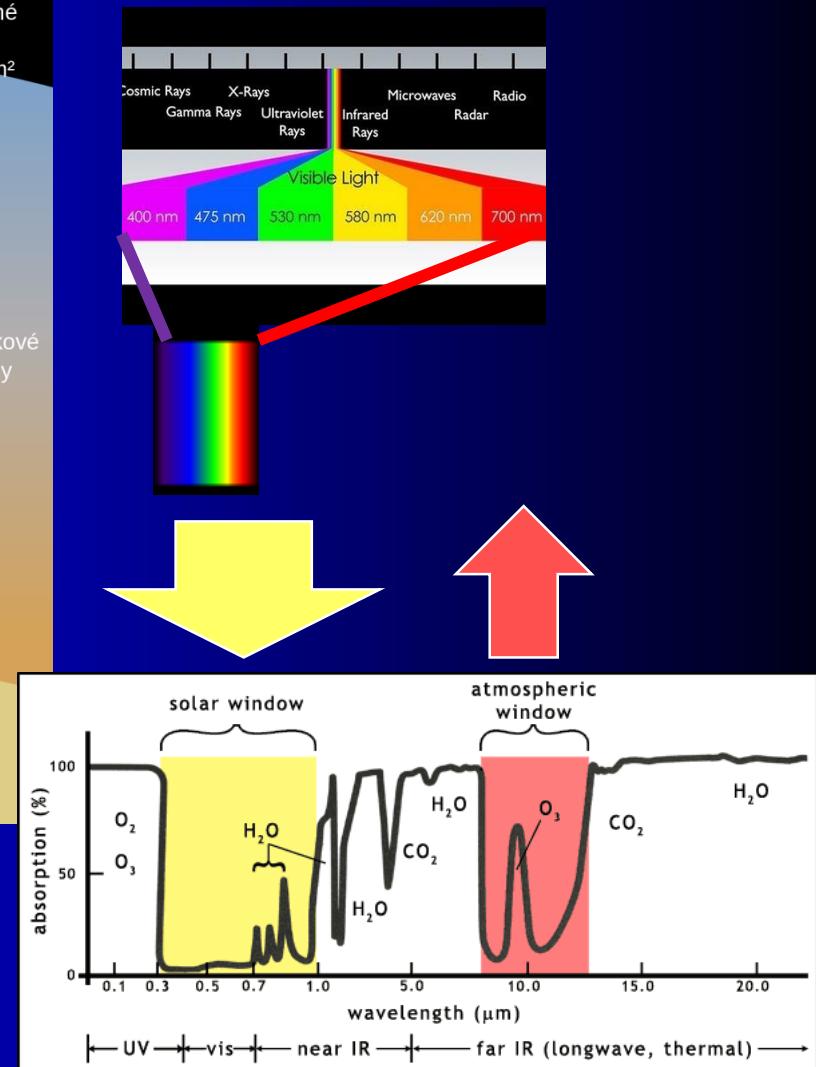
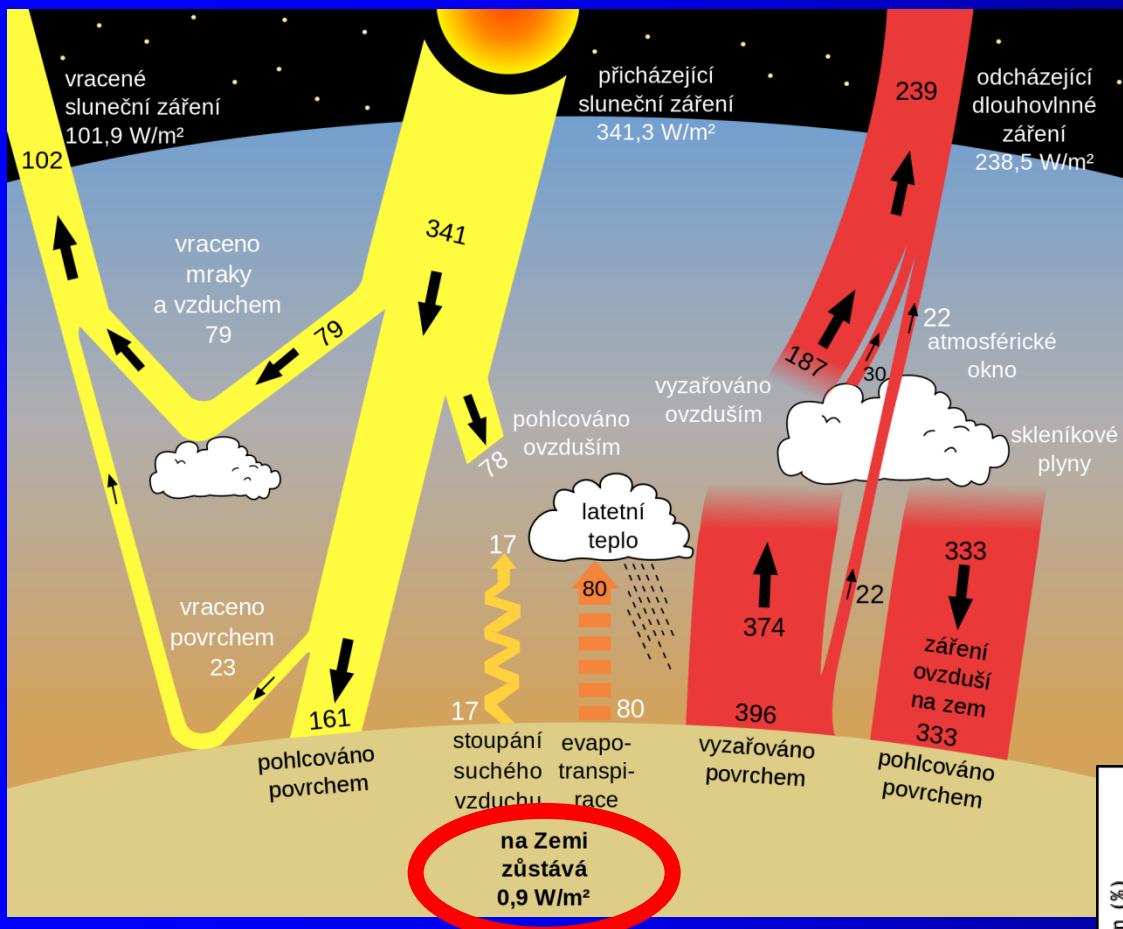
# Absorption



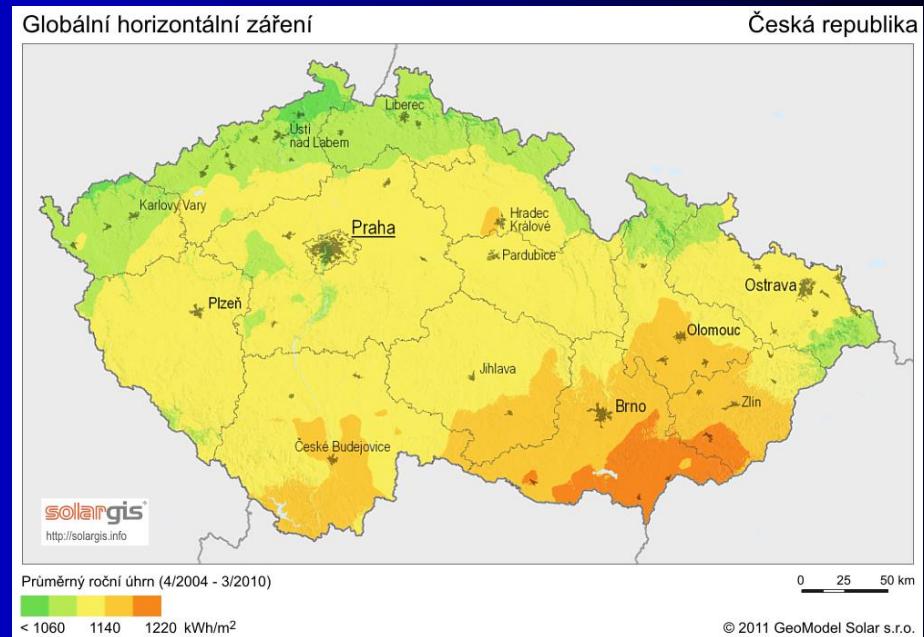
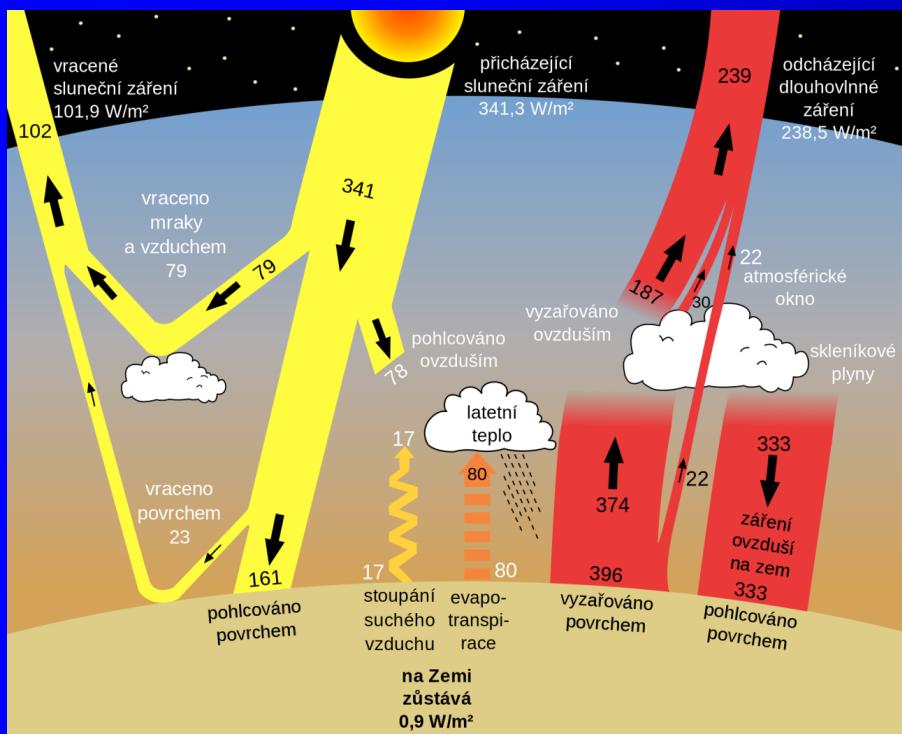
11 km

Ground level

# approximation



Krátkovlnné záření ze Slunce dopadající na zemský povrch a atmosféru. Dlouhovlnná část záření je emitována z povrchu a téměř zcela absorbována do atmosféry. V tepelné rovnováze je absorbovaná energie z atmosféry stejná jako ta vydávaná do vesmíru. Čísla ukazují výkon záření ve wattech na metr čtvereční v období let 2000–2004



.... elektřiny stanoven na **6 Kč/kWh s DPH**  
 .... plynu na **3 Kč/kWh s DPH**.

# Back to PLASMA PHYSICS

Kinetic energy of single particle

Temperature of the gas....

Temperature of plasma ....Electrons ..... Ions..... Neutrals

$$E \leftrightarrow kT$$

$$1\text{eV} \sim 11\ 604.5\ \text{K}$$

$$1\text{K} \sim 9 \times 10^{-5}\text{eV}$$

$$E \leftrightarrow 3/2 * kT$$

.....

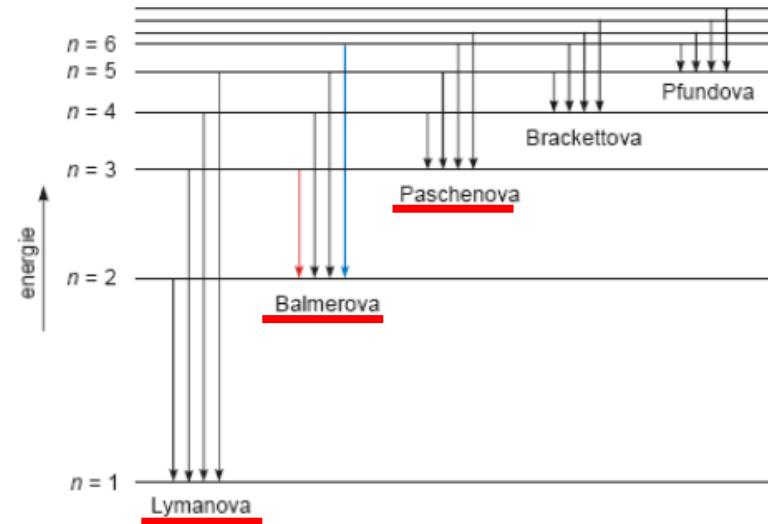
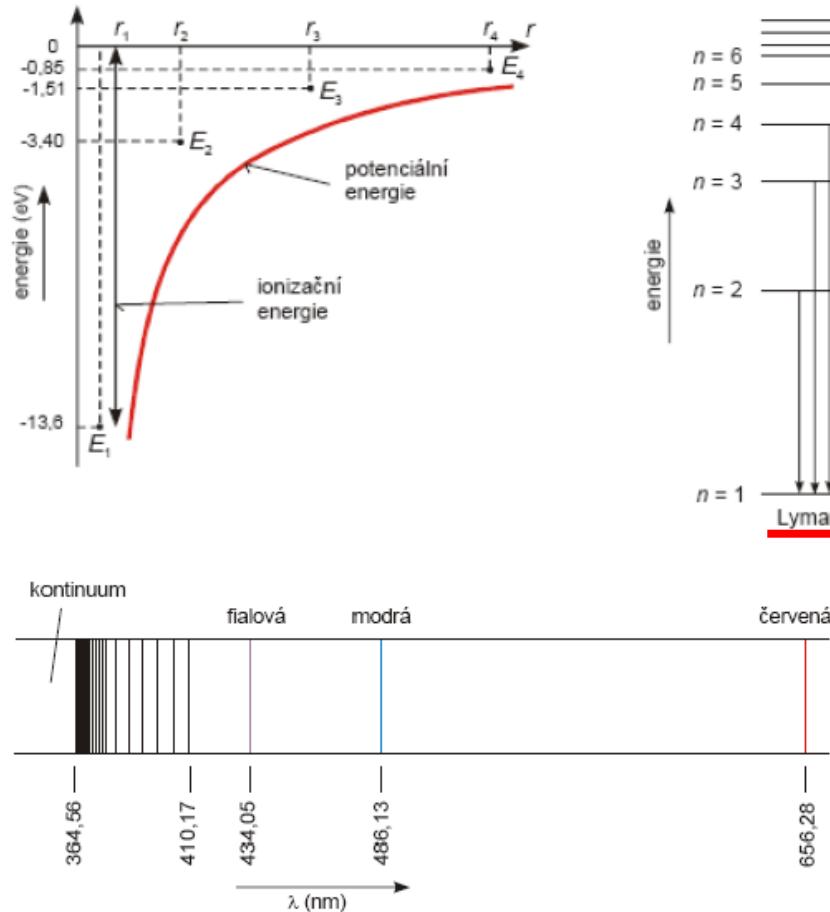
# Back to PLASMA PHYSICS



Niels Bohr

## Energy levels of H atom

### Spektrum atomu vodíku



$$h\nu = 13.6 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) [eV]$$

# Energy levels of H atom

Selection rule

$$\Delta l = \pm 1; \quad \Delta m_l = 0, \pm 1$$

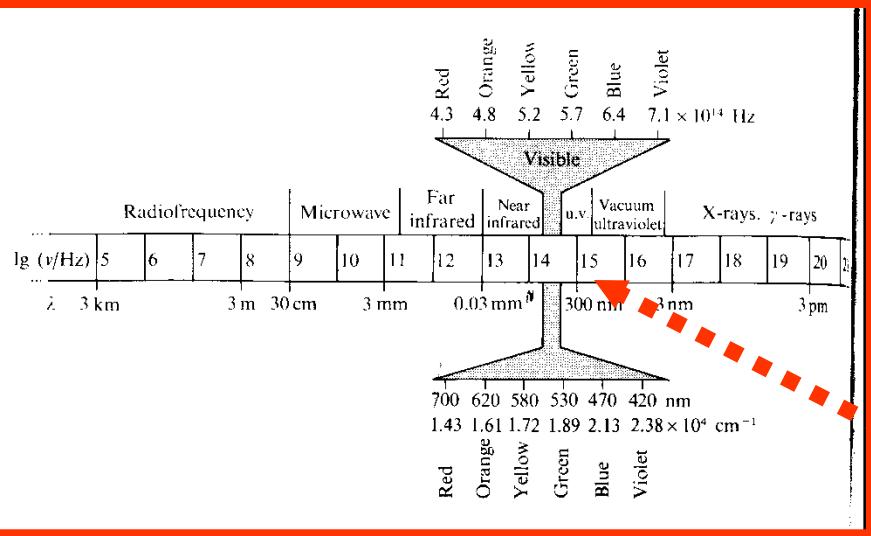
## Grotian diagram H

Angular momentum of photon is s=1

### 5.2 | Atomic structure and atomic spectra

**13.6eV**

Fig. 15.12. A Grotian diagram which summarizes the appearance and analysis of the spectrum of atomic hydrogen. The thicker the line, the more intense the transition.



$$E_n = -\frac{Z^2 \mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \propto \frac{1}{n^2}$$

$$h\nu = 13.6 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) [eV]$$

$$13.6eV \times 8065,5 \text{ cm}^{-1} \rightarrow 109000 \text{ cm}^{-1} \rightarrow 91 \text{ nm}$$

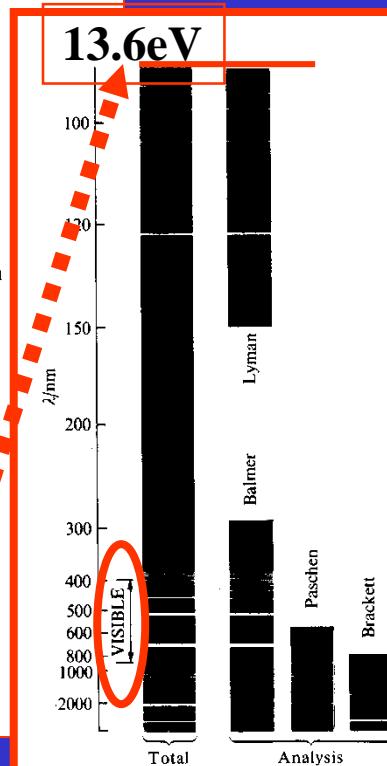
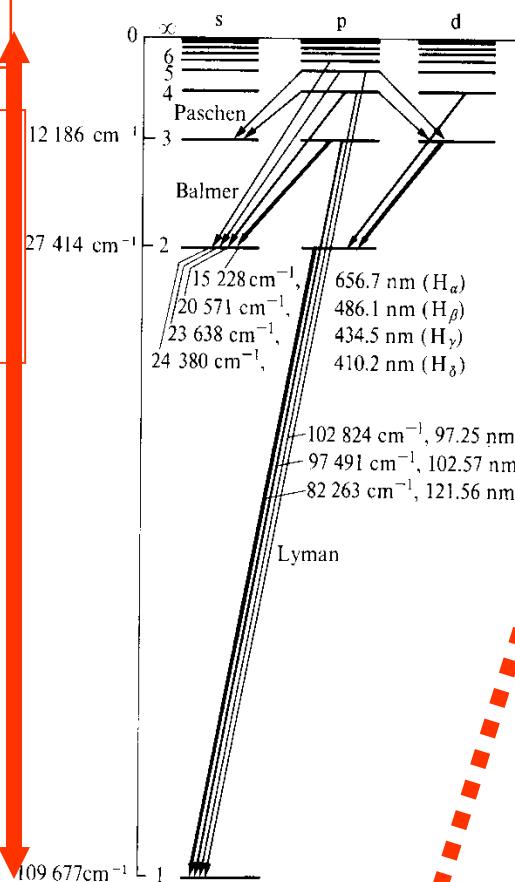
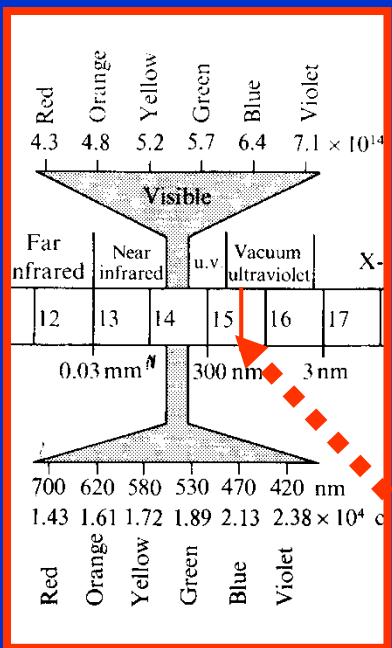


Fig. 15.1. The spectrum of atomic hydrogen. The spectrum is shown on the left, and is analysed into its overlapping series on the right. Note that the Balmer series lies in the visible region.

# Energy levels of He



Grotian diagram He  
Ionization energy He

24.46eV

He ionization energy

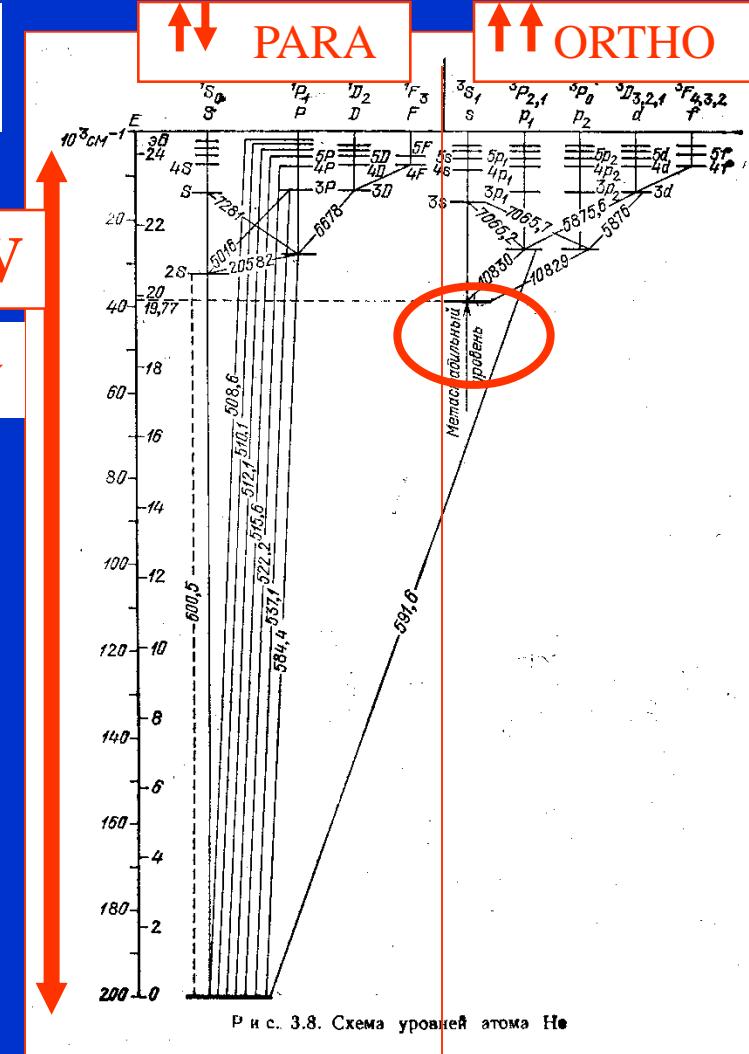
24.46eV  $\rightarrow$   $\sim 198400 \text{ cm}^{-1} \rightarrow \sim 50 \text{ nm}$   
vacuum ultraviolet

He<sup>+</sup> ionization energy

$$E_n = -\frac{Z^2 \mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \times \frac{1}{n^2} = -4 \times \frac{\mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \times \frac{1}{n^2}$$

$$h\nu = 4 \times 13.6 \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) [\text{eV}]$$

He<sup>+</sup> ionization energy (to form He<sup>++</sup>) = 54.4 eV



Singlet

Triplet

Spin of electrons

# Rydberg atom

$$\langle r \rangle_{n,l} = n^2 \left\{ 1 + \frac{1}{2} \left( 1 - \frac{l(l+1)}{n^2} \right) \right\} x \frac{a_0}{Z}$$

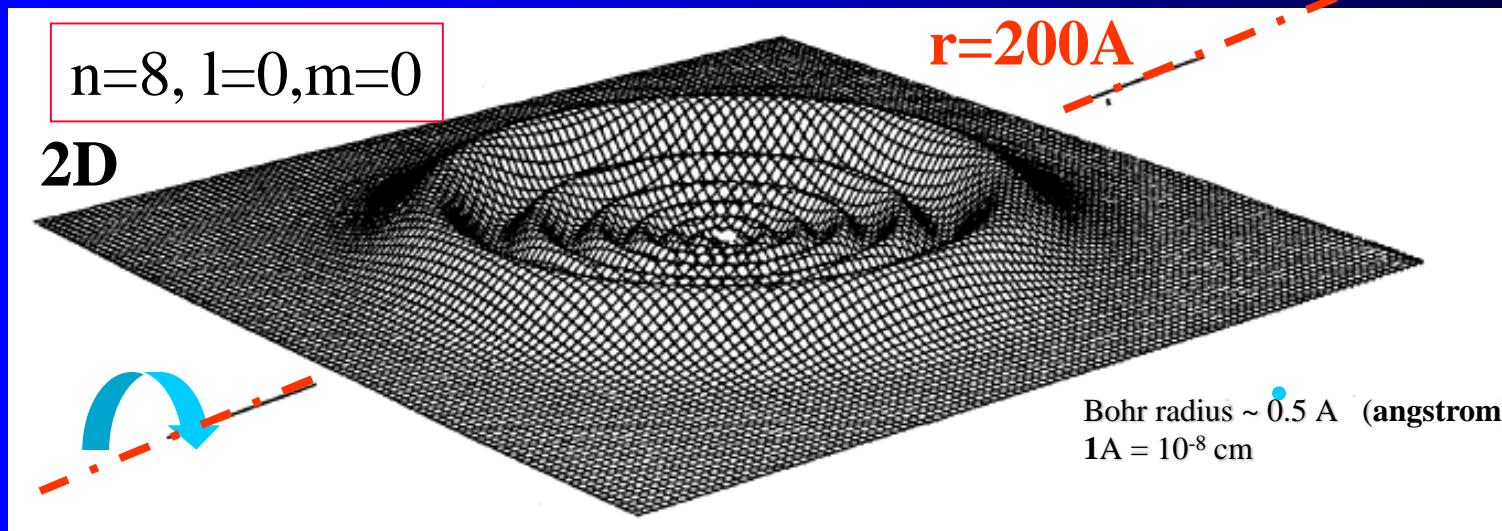
$$\langle r \rangle_{n,l=0} = n^2 \left\{ \frac{3}{2} \right\} x \frac{a_0}{Z}$$

## Highly Excited Atoms

*They are floppy, fragile and huge. Some of them have been found to have a diameter of almost a hundredth of a millimeter, which is 100,000 times the diameter of an atom in its lowest energy state*

by Daniel Kleppner, Michael G. Littman and Myron L. Zimmerman

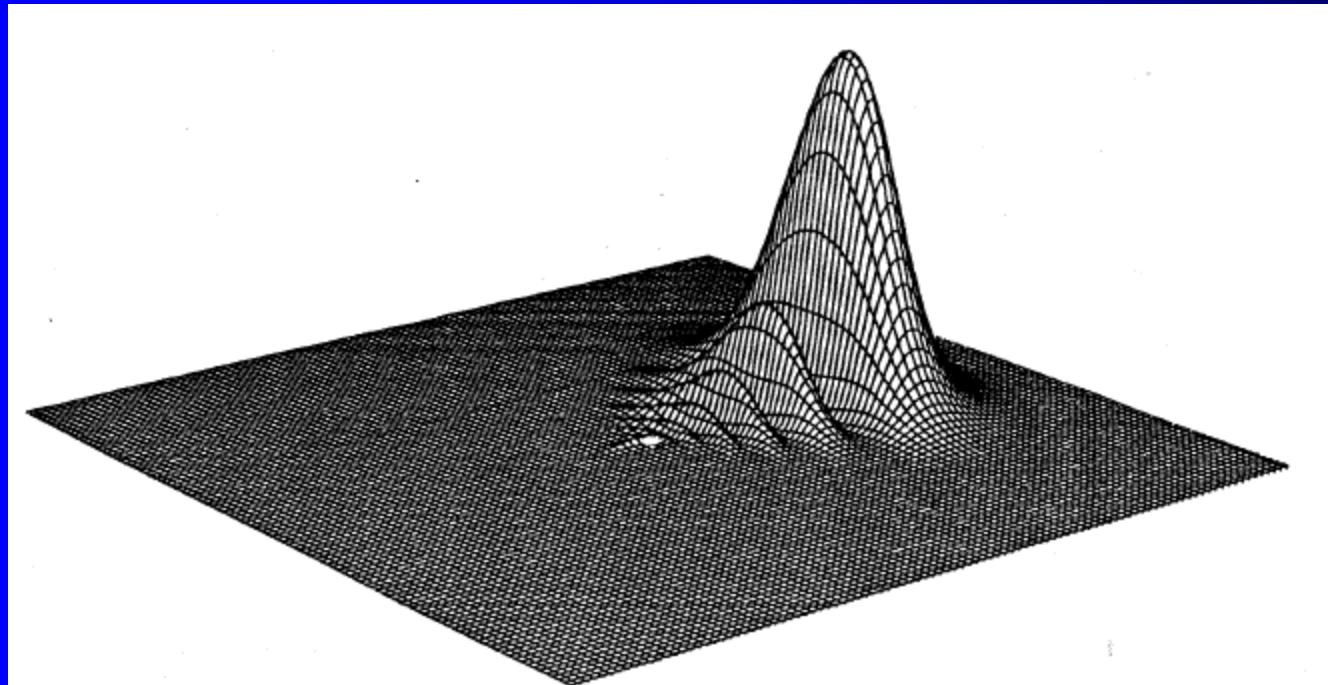
Bohr radius  $\sim 0.5 \text{ \AA}$  (angstrom)  
 $1\text{\AA} = 10^{-8} \text{ cm}^{-1}$



ELECTRON-CHARGE DENSITY OF HYDROGEN is graphed on a plane passing through the single proton that forms the nucleus of the atom (colored dot). The states of hydrogen are described by the three quantum numbers  $n$ ,  $l$  and  $m$ ;  $n$  is a positive integer that designates the energy level of the electron,  $l$  is an integer between 0 and  $n-1$  that corresponds to the magnitude of the eccentricity (or angular momentum) of the electron's orbit and  $m$  is an integer between  $-l$  and  $+l$  that describes the orbit's orientation. In the state where  $n=8$ ,  $l=0$  and  $m=0$  (upper graph) charge density is a series of concentric wavelike peaks. In three dimensions the charge density can be visualized as a series of spherical shells formed by rotating the graph about an axis passing through the nucleus. The distance from the nu-

cleus to the edge of the plane corresponds to  $2 \times 10^{-6}$  centimeter, which is 380 times the Bohr radius (the radius of a hydrogen atom in the lowest energy state). In a weak electric field (lower graph) the electron in an  $n=8$  state of hydrogen "stands" far to one side of the proton, forming an electric dipole. (In this state  $m=0$  and the angular momentum is a mixture of all possible values of  $l$  from zero to 7.) A dipole consists of two equal and opposite charges separated by a fixed distance. Many atoms act as dipoles, but most of them are not true dipoles: there is no separation of charges but only a slight distortion of the charge cloud. In the diagrammed state the separation is real. An atom whose outermost electron has been excited to a high energy level is often called a Rydberg atom. All Rydberg atoms are true dipoles.

# Rydberg atom in electric field



$n=8, l=0, m=0$

**All Rydberg atoms are true dipoles.**

# Properties of Rydberg atoms

Table 1. Properties of Rydberg atoms.

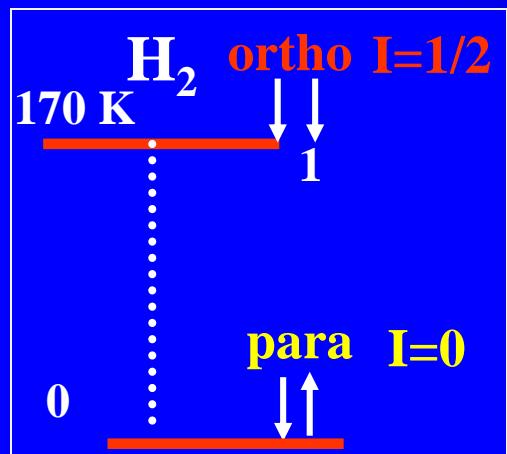
Property	$n$ dependence	Numerical values			
		$n=1$	$n=10$	$n=100$	$n=1000$
Bohr radius	$n^2 a_0$	$5.3 \times 10^{-9}$ cm	$5.3 \times 10^{-7}$ cm	$5.3 \times 10^{-5}$ cm	$5.3 \times 10^{-3}$ cm
Binding energy	$R/n^2$	13.6 eV	136 meV	1.36 meV	13.6 $\mu$ eV
RMS velocity of Rydberg electron	$v_0/n$	$2.2 \times 10^8$ cm s <sup>-1</sup>	$2.2 \times 10^7$ cm s <sup>-1</sup>	$2.2 \times 10^6$ cm s <sup>-1</sup>	$2.2 \times 10^5$ cm s <sup>-1</sup>
Orbital period	$n^3 \tau$	$1.5 \times 10^{-16}$ s	$1.5 \times 10^{-13}$ s	$1.5 \times 10^{-10}$ s	$1.5 \times 10^{-7}$ s
Classical field ionization threshold	$\frac{1}{16} n^4$	$3.2 \times 10^8$ V cm <sup>-1</sup>	$3.2 \times 10^4$ V cm <sup>-1</sup>	3.2 V cm <sup>-1</sup>	$3.2 \times 10^{-4}$ V cm <sup>-1</sup>

Bohr radius  $\sim 0.5 \text{ \AA}$  (angstrom)

$$1 \text{ \AA} = 10^{-8} \text{ cm}^{-1}$$

Small differences in zero point energies ....  
not sufficient to describe IMR @ low T  
nuclear spin selection rules

$$E \leftrightarrow kT$$
$$1\text{eV} \sim 11\,604.5 \text{ K}$$
$$1\text{K} \sim 9 \times 10^{-5} \text{ eV}$$



Energy levels  
Rotational states

## Energies of $H_2$ and $D_2$

$H_2$

$B_e=60.80$

$D_2$

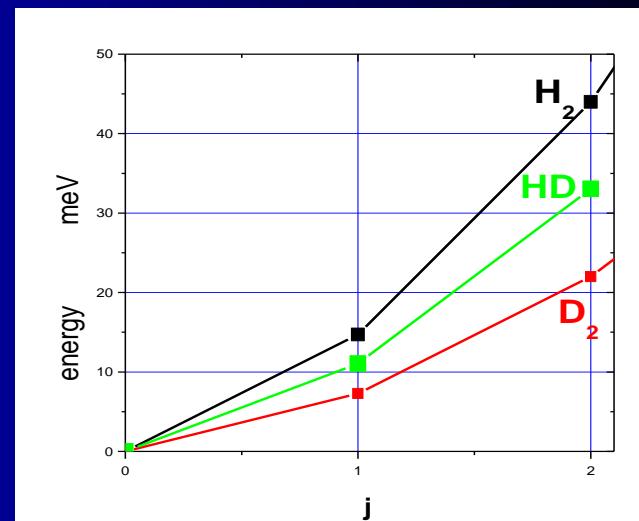
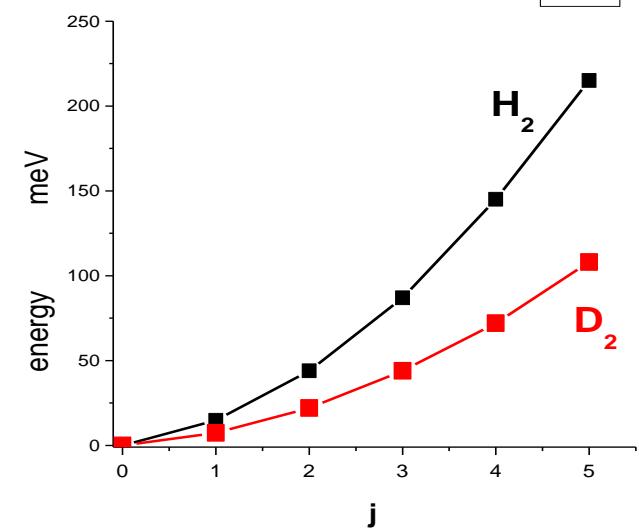
$B_e=30.429$

HD

$B_e=45.655$

1eV corresponds to  $\sim 11604K$

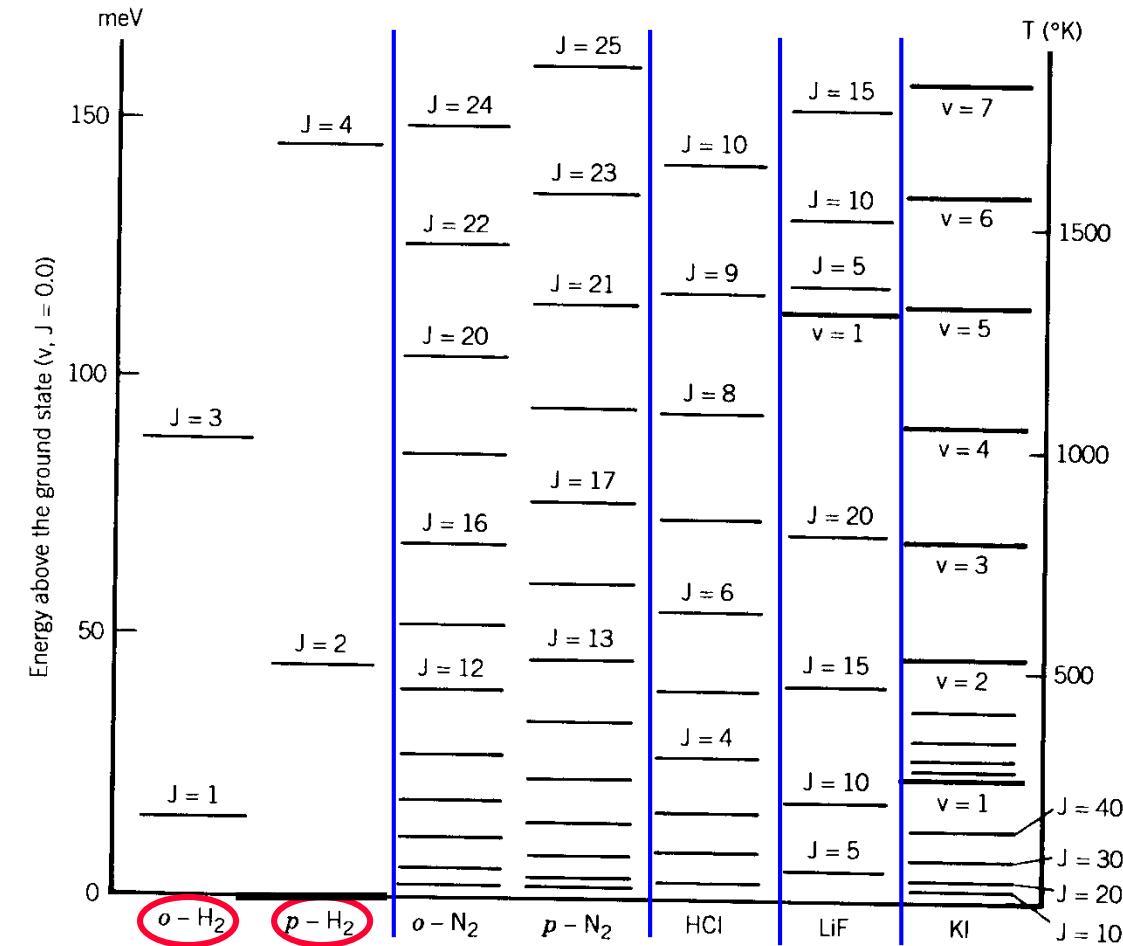
j	E/meV	E/in K	300K	250K	80K	35K	low
$H_2$	0	0	0.128	0.150	0.248	0.25	1/4
	1	14.7	170.6	0.657	0.694	0.75	3/4
	2	44	510.6	0.117	0.098	0.002	0
	3	87	1009.5	0.092	0.055	0	0
	4	145	1682.6	0.004	0.0016	0	0
	5	215	2494.9	0.001	0.0002	0	0
$D_2$	0	0	0.179	0.213	0.552	0.664	2/3
	1	7.3	84.71	0.202	0.227	0.329	0.333
	2	22	255.29	0.383	0.384	0.114	0.002
	3	44	510.6	0.115	0.098	0.004	0
	4	72	835.5	0.098	0.066	0.0001	0
	5	108	1253.2	0.015	0.008	0	0
HD	0	0	0	0	0	0	1
	1	11.04	128.1	0	0	0	0
	2	33.05	383.4	0	0	0	0



$H_2$  and  $D_2$  are taken from O. Wick dissertation

HD is calculated using  $B_e$  from Herzberg and comparison with  $H_2$  from table

# Energy levels Rotational states



**Figure 2-2-1.** Vibrational-rotational levels (quantum numbers  $v$  and  $J$ ) of a few diatomic molecules. The ( $v = 1, J = 0$ ) level of H<sub>2</sub> lies 0.54 eV above the ground state ( $v = 0, J = 0$ ). Rotational level spacings for H<sub>2</sub> are uniquely large, about  $15J$  meV, where  $J$  is the quantum number for the upper level. For the ortho species of H<sub>2</sub>(*o*-H<sub>2</sub>), the nuclear spins are parallel; for the para version (*p*-H<sub>2</sub>), the nuclear spins are antiparallel. [From Shimamura (1984).]

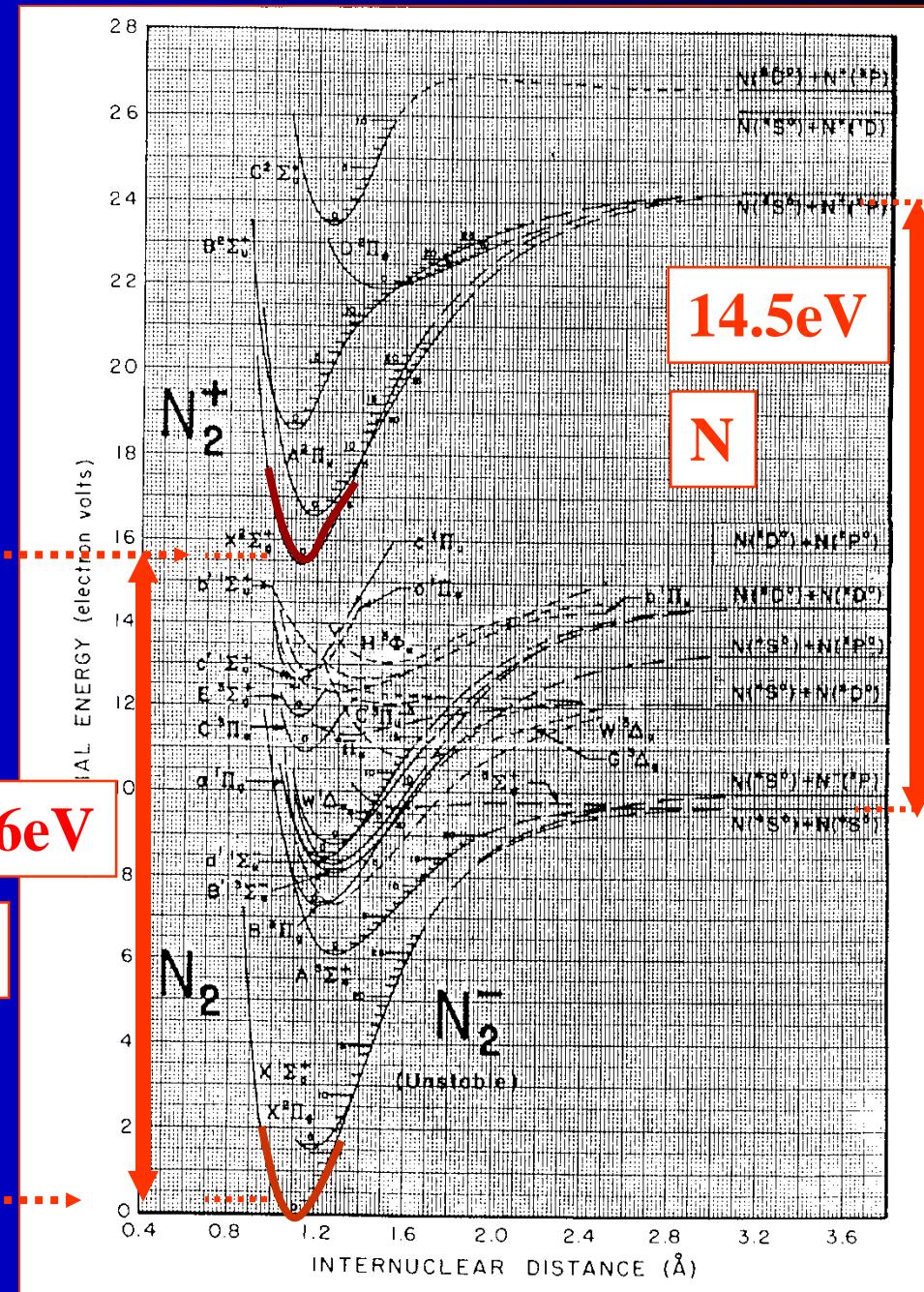
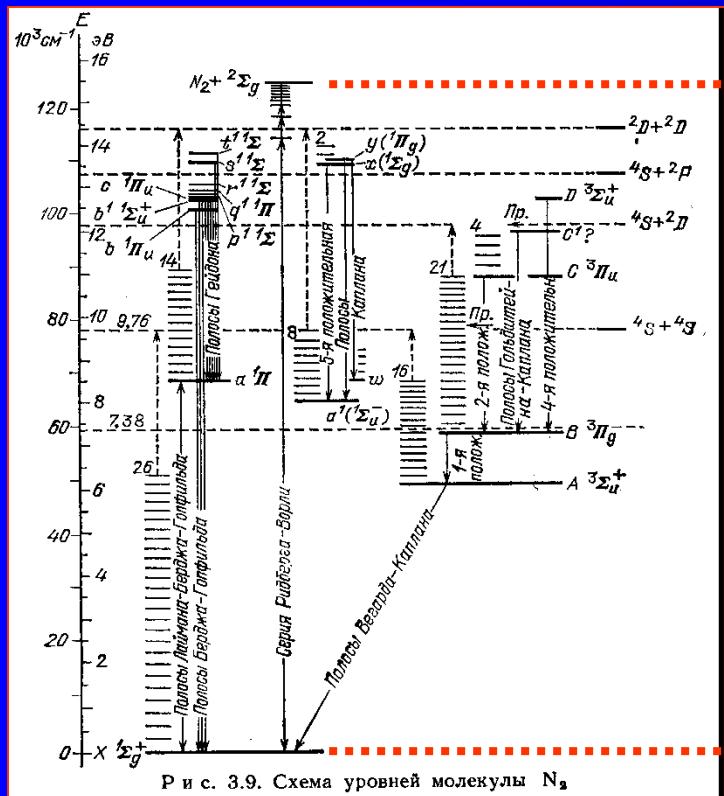
**$E \leftrightarrow kT$**   
**1eV ~ 11 604.5 K**  
**1K ~  $9 \times 10^{-5}$ eV**

## Potential curves $N_2$ , $N_2^+$

# Vibrational states

# Electronic states

# Ionisation



# Information

## Classical or quantum approach?

### Electron:

1eV →

$$v = 5.9 \times 10^7 \text{ cm s}^{-1}$$

$$\tau \sim a_0/v \sim 10^{-8} / 5.9 \times 10^7 = 2 \times 10^{-16} \text{ s}$$

$$\lambda \sim 2A = 2 \times 10^{-8} \text{ cm de Broglie}$$

za 1μs..... 1μs x  $5.9 \times 10^7 \text{ cm s}^{-1} = 59 \text{ cm}$

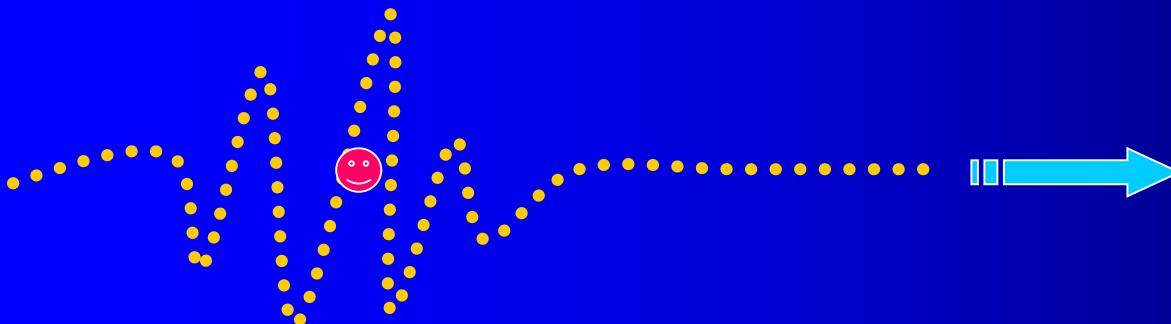
### Ar+:

1eV →

$$v = 2 \times 10^5 \text{ cm s}^{-1}$$

$$\tau \sim a_0/v \sim 10^{-8} / 2 \times 10^5 \sim 6 \times 10^{-14} \text{ s}$$

$$\lambda \sim 9 \times 10^{-11} \text{ cm de Broglie}$$

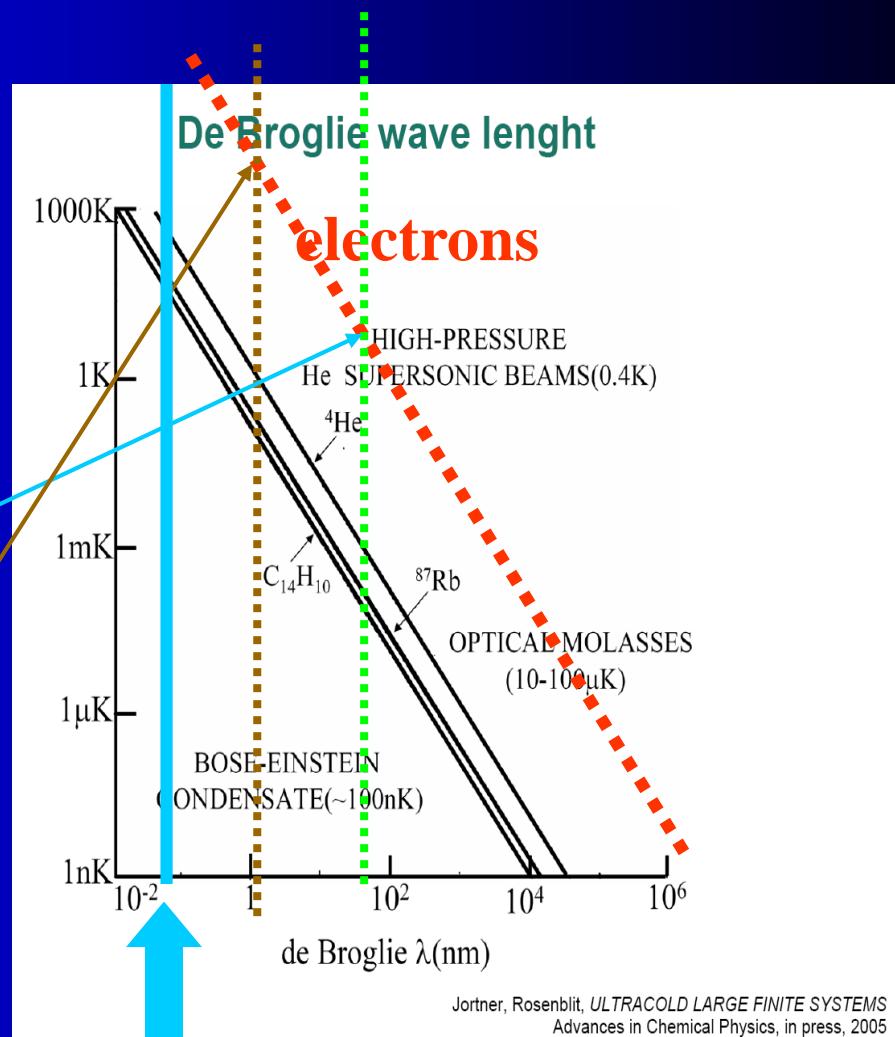


# De Broglie wave length

$$\lambda = \frac{h}{p} = \frac{h}{mv} \sqrt{1 - \frac{v^2}{c^2}}$$

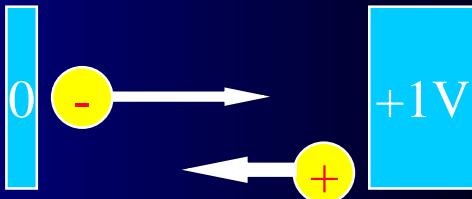
$$\lambda_e(4K) \sim 540 \text{ Å} \sim 54 \times 10^{-9} \text{ m}$$

$$\lambda_e(1eV) \sim 11.6 \text{ Å} \sim 1.16 \times 10^{-9} \text{ m}$$



# Electronvolt

$E \leftrightarrow kT$   
 $1\text{eV} \sim 11\,604.5\text{ K}$   
 $1\text{K} \sim 9 \times 10^{-5}\text{eV}$

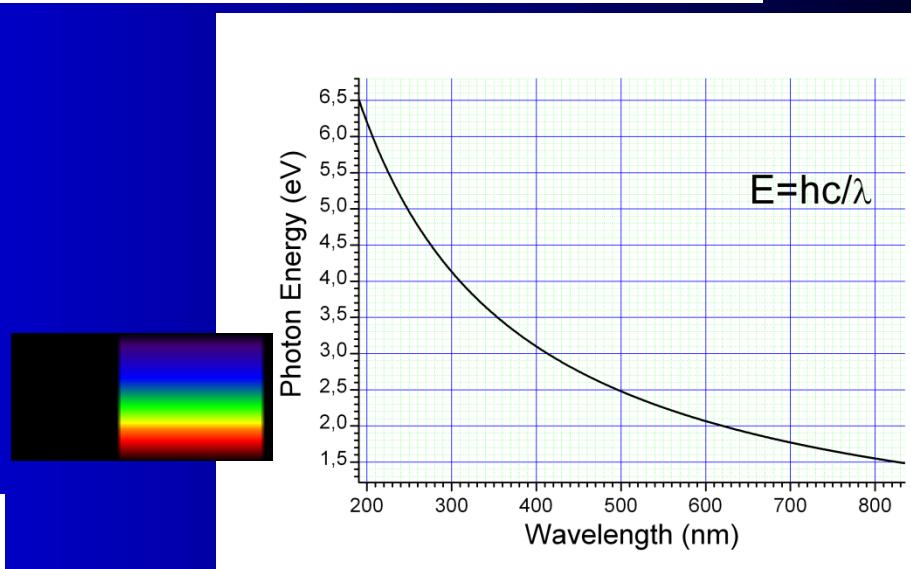


By definition, it is equal to the amount of kinetic energy gained by a single unbound electron when it accelerates through an electric potential difference of one volt

Conversion factors:

$1\text{ eV} = 1.6021765(40) \times 10^{-19}\text{J}$  (the conversion factor is numerically equal to the [elementary charge](#) expressed in [coulombs](#)).  
1 eV (per atom) is 96.485 [kJ/mol](#).

1.65 to 3.27 eV: the [photon energy](#) of visible light.



13.6 eV: The energy required to [ionize atomic hydrogen](#).  
[Molecular bond energies](#) are on the [order](#) of one eV per molecule

1 TeV: A trillion electronvolts, or  $1.602 \times 10^{-7}\text{ J}$ , about the kinetic energy of a flying [mosquito](#)

14 TeV: the design proton collision energy at the [Large Hadron Collider](#) (which has operated at half of the energy since March 30, 2010). ....

**Mol** (značka mol) je základní [fyzikální jednotka látkového množství](#).

Jeden mol libovolné látky obsahuje stejný počet [častic](#), jaký je obsažen [atomů](#) v 12 g [nuklidu uhlíku](#). Tento počet udává [Avogadrova konstanta](#), jejíž hodnota je přibližně  $6,022 \times 10^{23}\text{ mol}^{-1}$ .

# Conversion factors

$$1 \text{ eV}/k = \frac{1 \text{ eV}}{8,617\,333\,262 \times 10^{-5} \text{ eV/K}} = 11\,604,518\,12\dots \text{ K}$$

$E \leftrightarrow kT$

$1 \text{ eV} \sim 11\,604.5 \text{ K}$

$1 \text{ K} \sim 9 \times 10^{-5} \text{ eV}$

Atkins  
Physical chemistry



$$R\mathcal{F} = 2.4789 \text{ kJ mol}^{-1}$$

$$R\mathcal{F}/F = 25.693 \text{ mV}$$

$$2.3026 R\mathcal{F}/F = 59.159 \text{ mV}$$

$$k\mathcal{F}/hc = 207.223 \text{ cm}^{-1}$$

$$V_m^\ominus = R\mathcal{F}/p^\ominus = 2.4465 \times 10^{-2} \text{ m}^3 \text{ mol}^{-1} = 24.465 \text{ dm}^3 \text{ mol}^{-1}$$

$T/\text{K}$	100.00	298.15	500.00	1000.0	1500.0	2000.0
$(kT/ke)/\text{cm}^{-1}$	69.50	207.22	347.51	659.03	1042.5	1390.1

$$p^\ominus = 100 \text{ kPa} = 1 \times 10^5 \text{ N m}^{-2}$$

$$1 \text{ atm} = 101.325 \text{ kPa} = 1.013\,25 \times 10^5 \text{ N m}^{-2} = 1.013\,25 \times 10^5 \text{ J m}^{-3}$$

$$1 \text{ atm} = 760 \text{ Torr} \text{ (exactly)}$$

$$1 \text{ Torr} = 133.322 \text{ Pa} \text{ (exactly)}$$

$$1 \text{ mmHg} = 133.3224 \text{ Pa}$$

$$1 \text{ eV} = 1.602\,19 \times 10^{-19} \text{ J} \triangleq 96.485 \text{ kJ mol}^{-1} \triangleq 8065.5 \text{ cm}^{-1}$$

$$1 \text{ cm}^{-1} \triangleq 1.986 \times 10^{-23} \text{ J} \triangleq 11.96 \text{ J mol}^{-1} \triangleq 0.1240 \text{ meV}$$

$1 \text{ eV} \approx 23.06 \text{ hc}$

$$hc = 1.986\,48 \times 10^{-23} \text{ J cm}$$

$$hc/k = 1.438\,79 \text{ cm K}$$

$$g/\text{m s}^{-2} = 9.8064 - 0.0259 \cos \{2(\text{latitude})\} = 9.811 \text{ at } 50^\circ$$

$$1 \text{ cal} = 4.184 \text{ J}$$

$$1 \text{ D (debye)} = 3.335\,64 \times 10^{-30} \text{ C m}$$

$$1 \text{ N} = 1 \text{ J m}^{-1} = 10^5 \text{ dyne}$$

$$1 \text{ W} = 1 \text{ J s}^{-1}$$

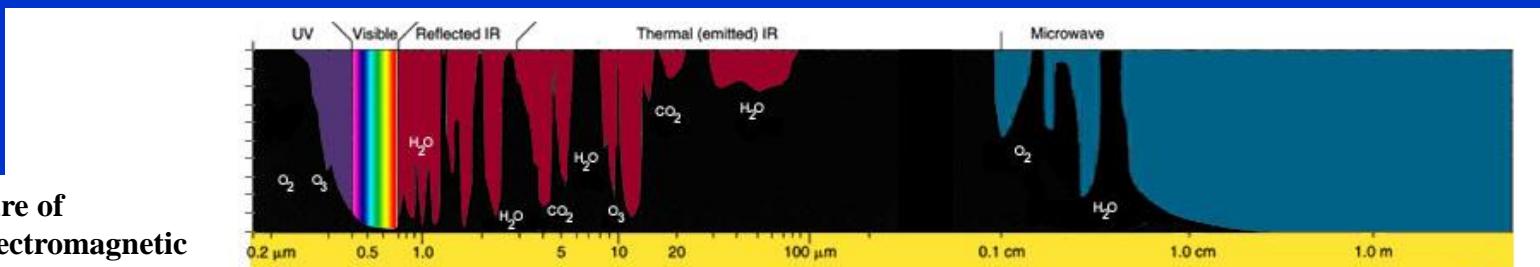
$$1 \text{ T} = 1 \text{ J C}^{-1} \text{ s m}^{-2}$$

$$1 \text{ J} = 10^7 \text{ erg}$$

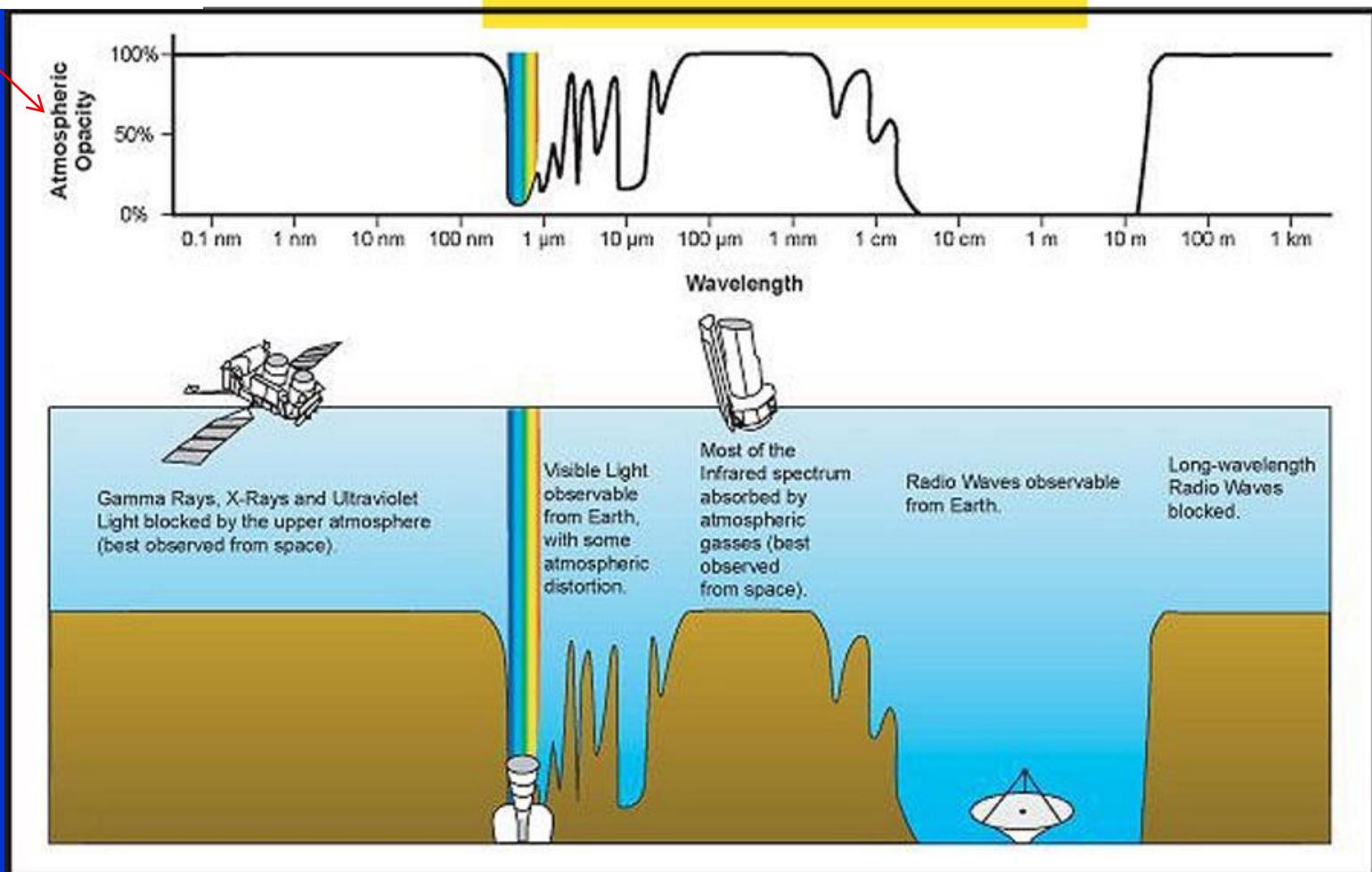
$$1 \text{ A} = 1 \text{ C s}^{-1}$$

$$1 \text{ J} = 1 \text{ A V s}$$

# Detail 0.1nm-1 km



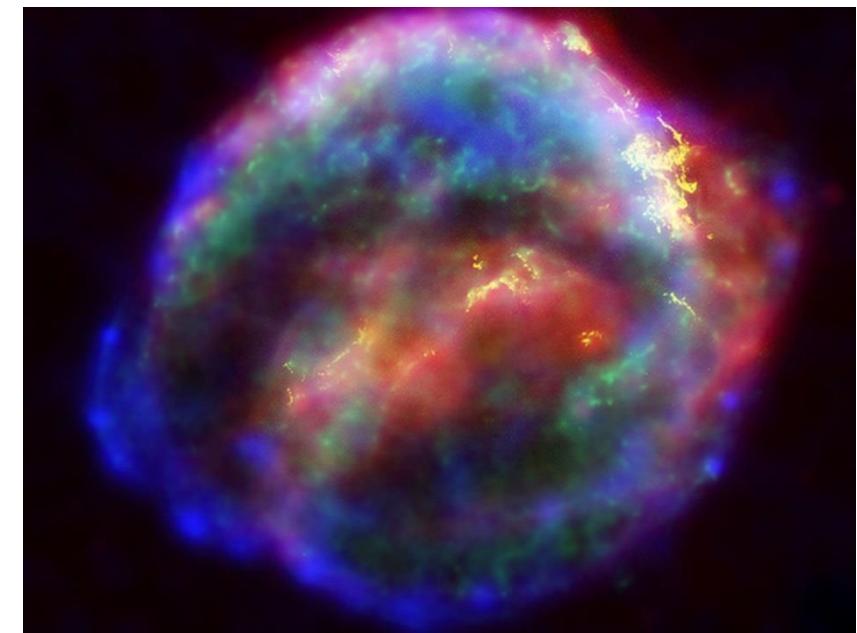
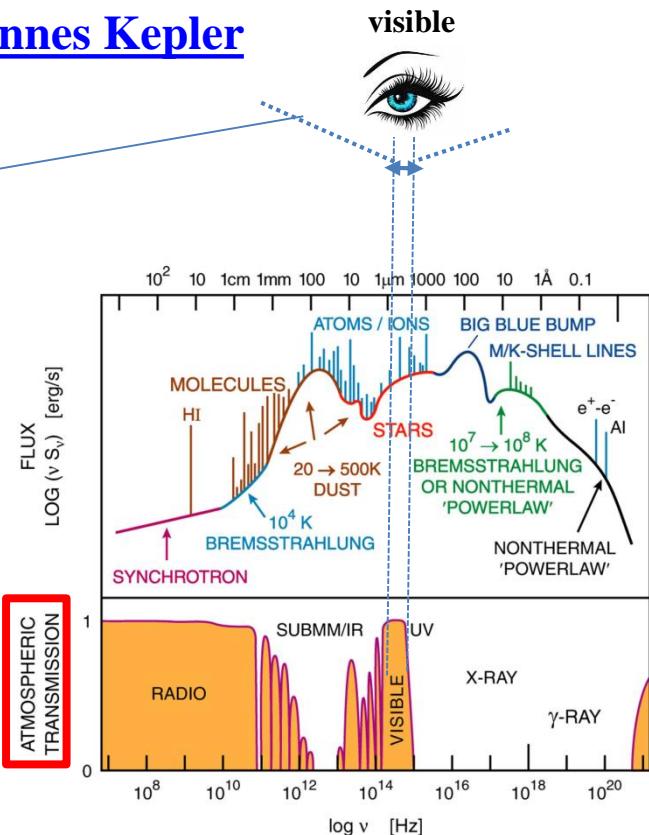
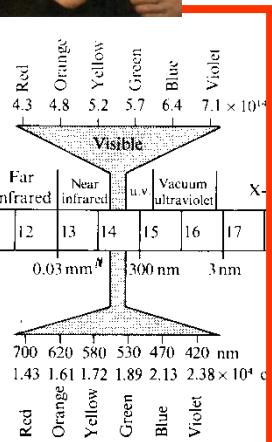
Opacity is the measure of impenetrability to electromagnetic or other kinds of radiation, especially visible light.



Before

## Johannes Kepler

The Supernova of 1604



The first recorded observation was in northern Italy on October 9, 1604.<sup>[2]</sup> Johannes Kepler began observing the luminous display while working at the imperial court in Prague for Emperor Rudolf II on October 17.<sup>[3]</sup> It was subsequently named after him because his observations tracked the object for an entire year and because of his book on the subject, entitled *De Stella nova in pede Serpentarii* ("On the new star in Ophiuchus's foot", Prague 1606).

It was the second supernova to be observed in a generation (after SN 1572 seen by Tycho Brahe in Cassiopeia). No further supernovae have since been observed with certainty in the Milky Way, though many others outside our galaxy have been seen since S Andromedae and SN 1987A in the Large Magellanic Cloud was visible to the naked eye.

Golden Age of Astro-plasma and Astro-chemistry

1722



## Klementinum and astronomy. Astronomická věž

1722



socha Atlanta



Věž byla dokončena v roce 1722. Na vrcholu věže stojí socha Atlanta (оловěná socha s železnou vnitřní konstrukcí, váha asi 600 kg, výška 2,4 m). Atlas nese nebeskou sféru (průměr asi 1,6 m, váha asi 150 kg) s korouhví.

(Pravděpodobně  
Matyáš Braun)

# Golden Age of Astrochemistry



Спутник

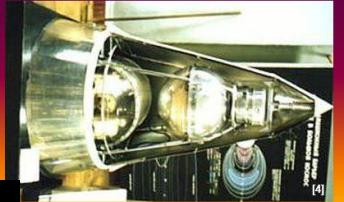
4. Oktober 1957 19:28 UTC

Družice měla sférický tvar o průměru 58 cm a hmotnost 83,6 kg.

## 1957 - PES LAJKA



- 3. listopadu 1957 vyslal Sovětský svaz na palubě družice Sputnik 2 na oběžnou dráhu prvního pozemského živého tvora – fenku Lajku.
- Zpátky na Zem se však nevrátila, protože to tehdejší technika ještě neuměla.



3. November 1957

Byla zkonstruována koncem 50. let 20. století Sergejem Koroljovem v Sovětském svazu. Byla vynesena 4. října 1957 19:28 UTC upravenou dvoustupňovou nosnou raketou R-7, která byla z vojenské verze pro kosmonautiku upravena a přejmenována na raketu Sputnik. Odstartovala z kosmodromu Bajkonur na území Kazašské SSR. Vypuštěna byla v rámci Mezinárodního geofyzikálního roku.<sup>[2]</sup> Patří do kategorie vědeckých družic.

Sputnik 2

Hmotnost 508 kg

Lajka

3. listopadu 1957 z kosmodromu Bajkonur.

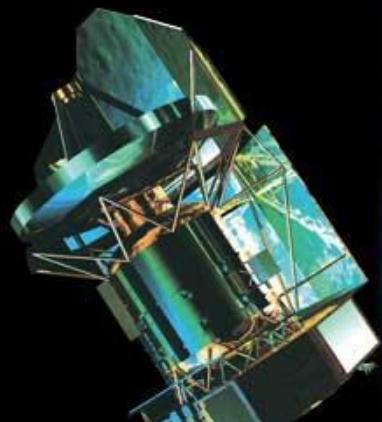
2021

~ 64 rokov

# Golden Age of Astrochemistry



Herschel

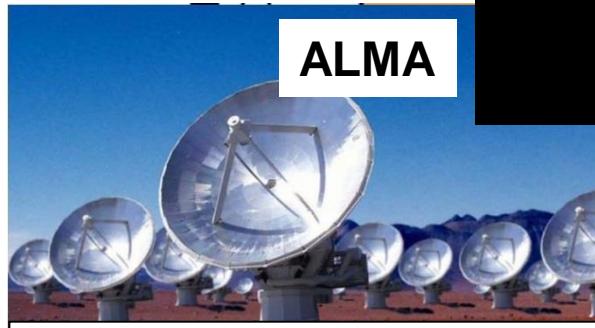
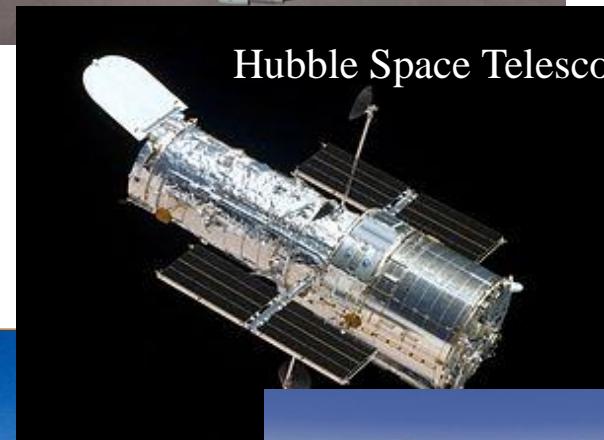


The Arecibo Observatory  
RT in [Puerto Rico](#) (~1960)

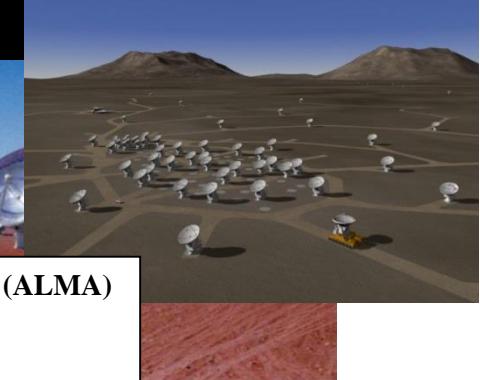


RATAN-600 Radio Telescope (Russia, 1974)

Five-hundred-meter Aperture Spherical radio  
Telescope (China: Tiyanan, 2016 )



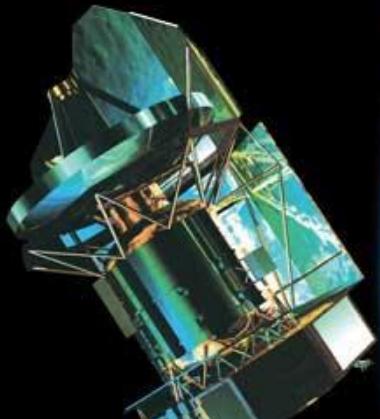
The Atacama Large Millimeter/sub-millimeter Array (ALMA)  
astronomical interferometer of radio telescopes  
Atacama desert of northern Chile



# Golden Age of Astrochemistry



Herschel



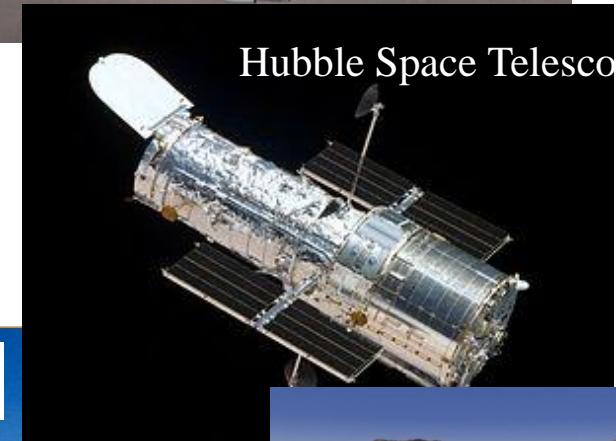
Five-hundred-meter Aperture Spherical radio Telescope (China: Tiyanan, 2016 )



SOFIA



The Arecibo Observatory  
RT in [Puerto Rico](#) (~1960)

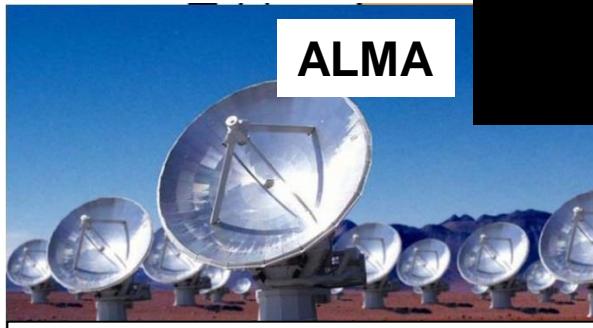


Hubble Space Telesco



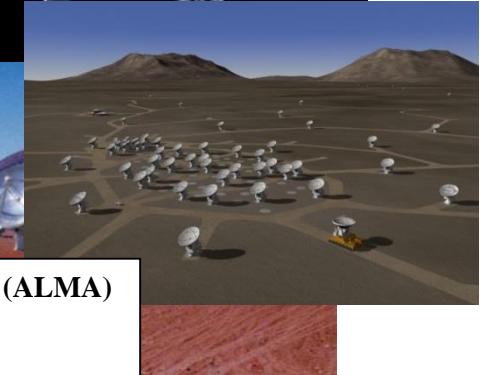
[Třetí nebeský palác](#)

Tiangong, officially the Tiangong space station

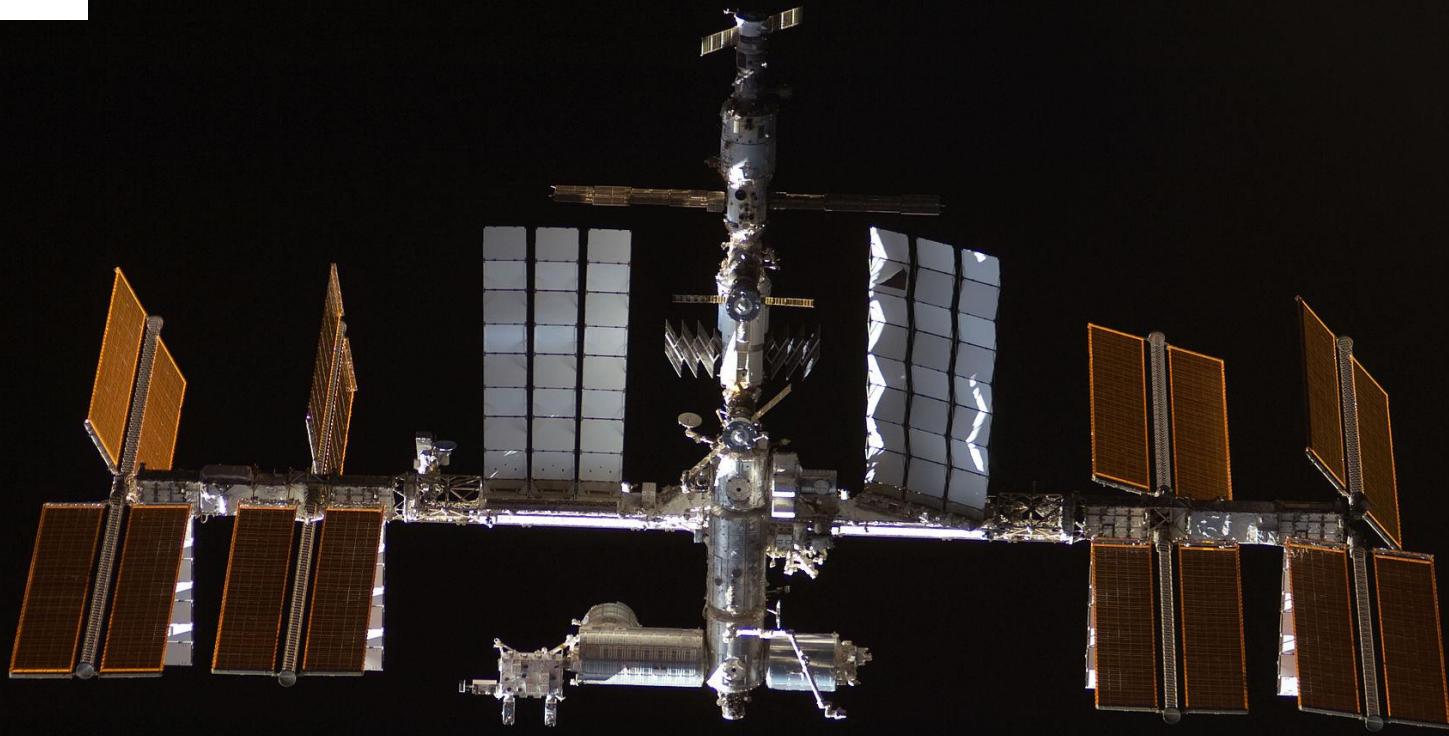


ALMA

The Atacama Large Millimeter/sub-millimeter Array (ALMA)  
astronomical interferometer of radio telescopes  
Atacama desert of northern Chile



**ISS**



## Hubble Space Telescope



From April 24, 1990

The Hubble Space Telescope is a space telescope that was launched into low Earth orbit in 1990 and remains in operation.

The telescope is operating as of 2019, and could last until 2030–2040.

Hubble is the only telescope designed to be maintained in space by astronauts. Five Space Shuttle missions have repaired, upgraded, and replaced systems on the telescope, including all five of the main instruments. The fifth mission was canceled on safety grounds following the [Columbia disaster](#) (2003), but NASA administrator [Michael D. Griffin](#) approved the [fifth servicing mission](#) which was completed in 2009. The telescope was still operating as of April 24, 2020, its 30th anniversary,<sup>[1]</sup> and could last until 2030–2040.<sup>[4]</sup> One successor to the Hubble telescope is the [James Webb Space Telescope](#) (JWST) which is scheduled to be launched in late 2021.<sup>[1]</sup>

## Not actualized, approximation

**Hubble má potíže, přestal fungovat čtvrtý gyroskop, který pomáhá s orientací teleskopu**

08. 10. 2018

### Hubble Teleskopy

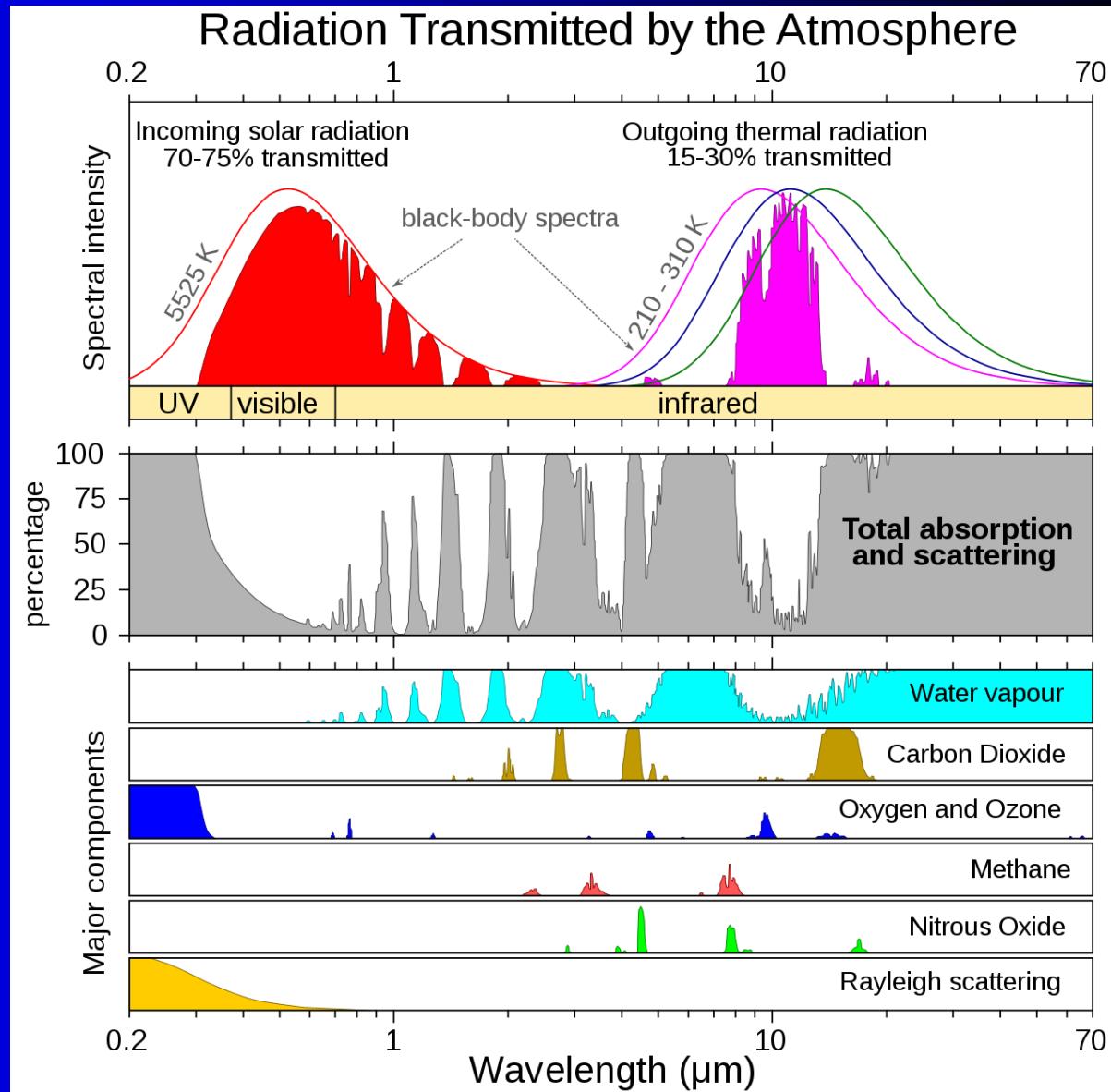
V pátek se vesmírný teleskop Hubble přepnul do tzv. safe módu poté, co přestal fungovat jeden z gyroskopů, které teleskopu pomáhají udržet správnou orientaci při pozorování vzdálených cílů ve vesmíru. Hubble měl celkem 6 těchto gyroskopů a potřebuje nejméně tří pro optimální operace. Dva však už delší dobu nefungují a další nefunguje optimálně. Po odchodu čtvrtého tak zbývají pouze dva funkční gyroskopy. Operátoři mise nyní zkoumají možnosti, kterými uvést teleskop zpátky do plného provozu.

Pokud se nepodaří na dálku opravit porouchaný gyroskop, hodlají operátoři vyzkoušet onen třetí, který nefunguje optimálně. Aktuálně tak hledají cesty, jak teleskop na dálku opravit, pokud se to nepodaří, teleskop může pracovat dál se dvěma, nebo dokonce jedním gyroskopem. Je dokonce pravděpodobné, že pokud se oprava nepodaří, mise bude dále pokračovat pouze s jedním gyroskopem a druhý bude ponechán jako rezerva.

Všechn šest gyroskopů teleskopu Hubble bylo vyměněno při poslední misi astronautů k teleskopu v roce 2009. Po dosloužení raketoplánů však teleskop nebyl astronauty navštíven a zatím se neplánuje žádná podobná mise s novými vesmírnými loděmi, které by NASA měla mít v následujících letech k dispozici. Hubble je ve vesmíru od roku 1990.

**Vesmírný teleskop Hubble** - teleskop Hubble obíhá Zemi od roku 1990 ve výšce asi 540 kilometrů.

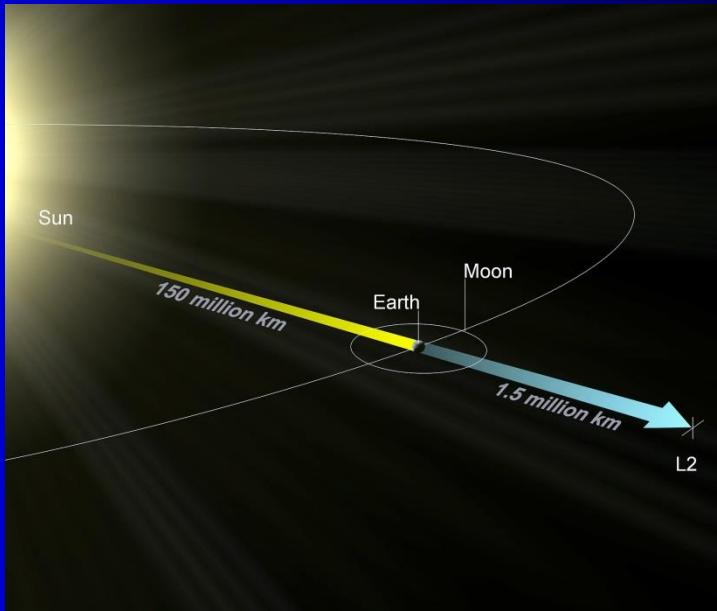
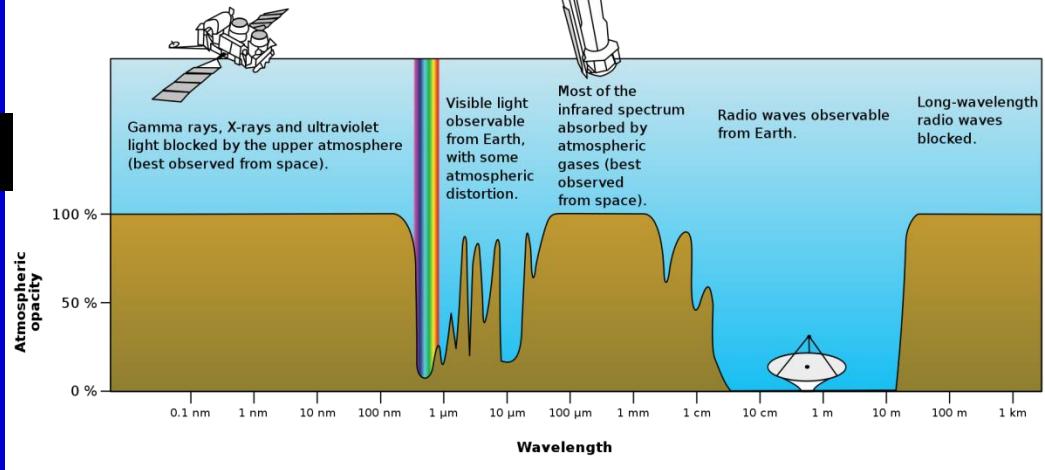
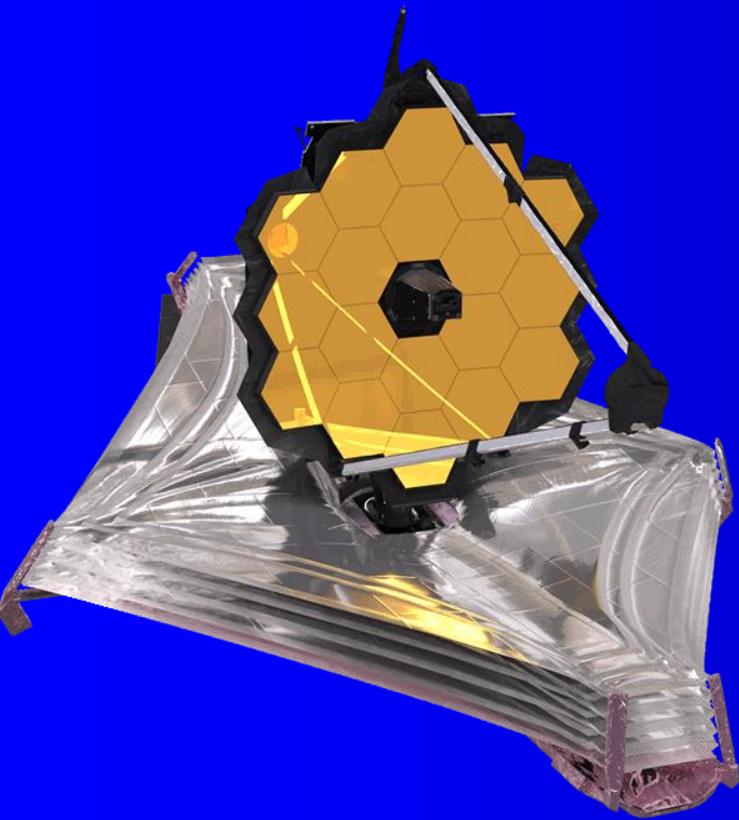
# James Webb Space Telescope



Atmospheric windows in the infrared: Much of this type of light is blocked when viewed from the Earth's surface. It would be like looking at a rainbow but only seeing one colour.

## infrared astronomy

### James Webb Space Telescope (JWST)



The **James Webb Space Telescope (JWST)** is a space telescope which conducts infrared astronomy. As the largest optical telescope in space, its high resolution and sensitivity allow it to view objects too old, distant, or faint for the Hubble Space Telescope. This will enable investigations across many fields of astronomy and cosmology, such as observation of the first stars, the formation of the first galaxies, and detailed atmospheric characterization of potentially habitable exoplanets.

$\sim$ 1/6 of mass is interstellar

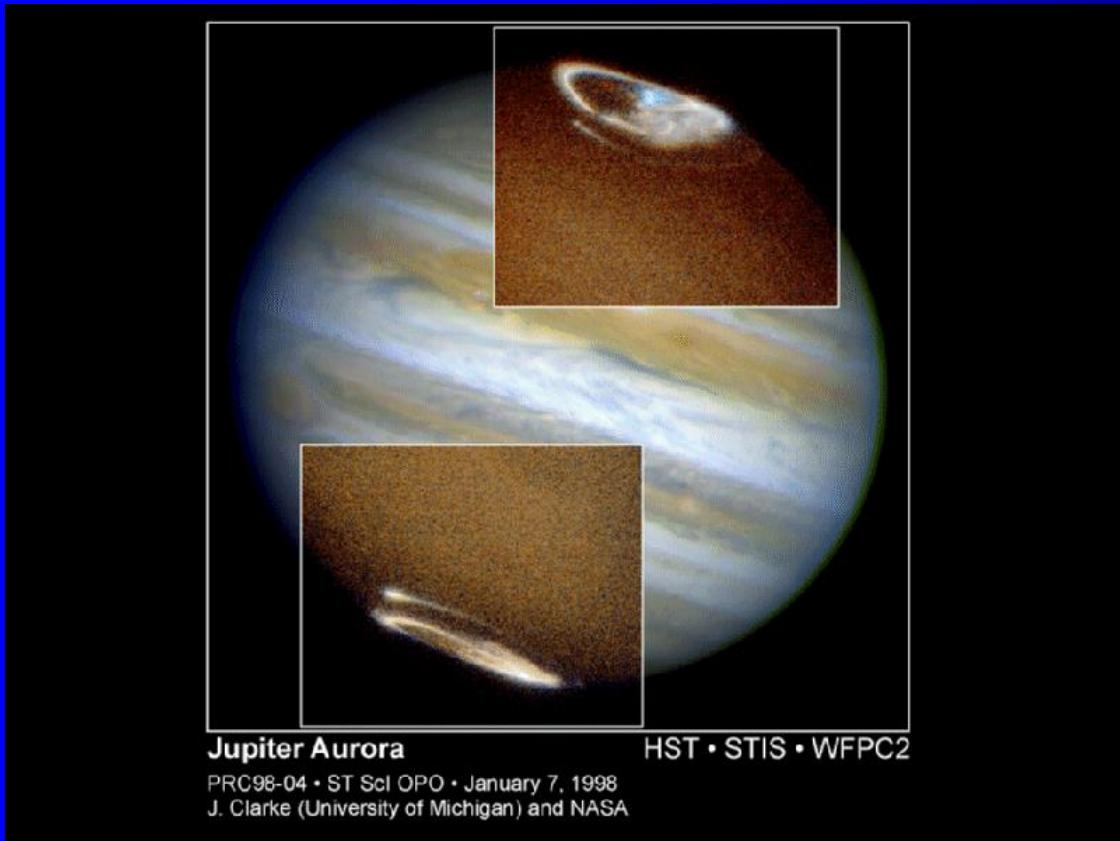
$\sim$ 1/2 of interstellar matter is molecular!



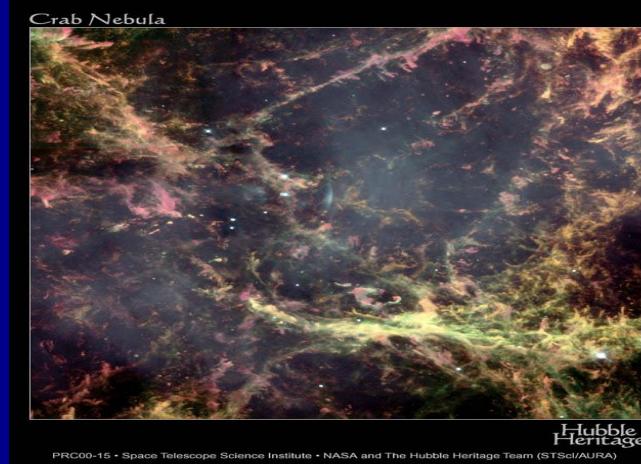
Milky Way has  $\sim 10^{66}$  molecules!  
Earth has only  $\sim 10^{50}$  molecules

Different views of the Milky Way (different wavelengths)

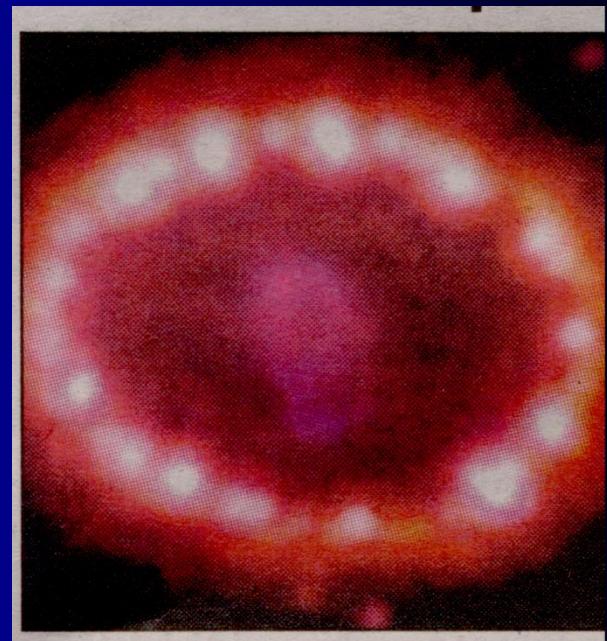
# Hydrogen dominated plasma



Hydrogen plasma in Jupiter Aurora

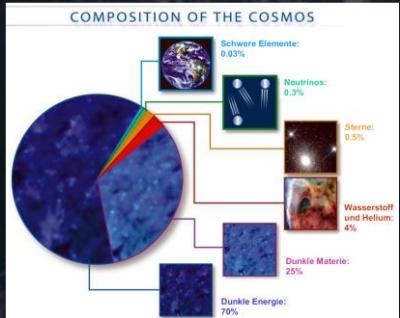


Crab Nebula



1994 -Supernova 1987A

## Formation of ions in interstellar space , laboratory astrophysics



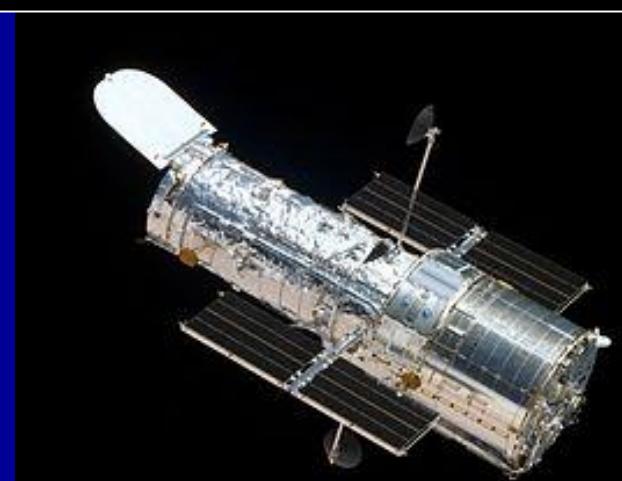


The **Crab Nebula** is the remnant of a supernova explosion that was observed by Chinese astronomers in the year 1054.



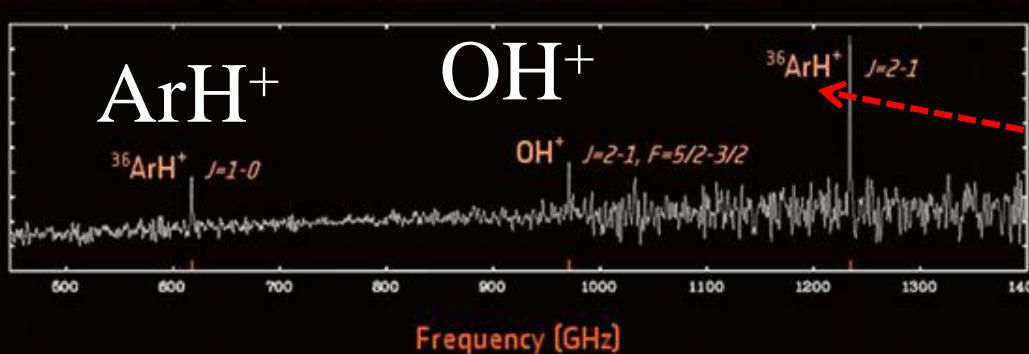
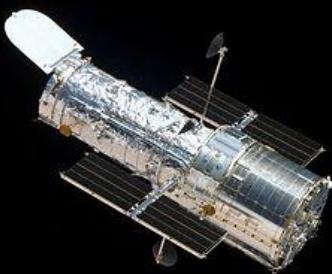
Herschel

Herschel (red) and Hubble (blue) composite image of the Crab Nebula. *Credit: ESA/Herschel/PACS/MESS Key Programme Supernova Remnant Team; NASA, ESA and Allison Loll/Jeff Hester (Arizona State Uni)*



Hubble Space Telescope

12 December 2013



Using ESA's Herschel Space Observatory, a team of astronomers has found first evidence of a noble-gas based molecule in space. A compound of argon, the molecule was detected in the gaseous filaments of the Crab Nebula, one of the most famous supernova remnants in our Galaxy. While argon is a product of supernova explosions, the formation and survival of argon-based molecules in the harsh environment of a supernova remnant is an unforeseen surprise.

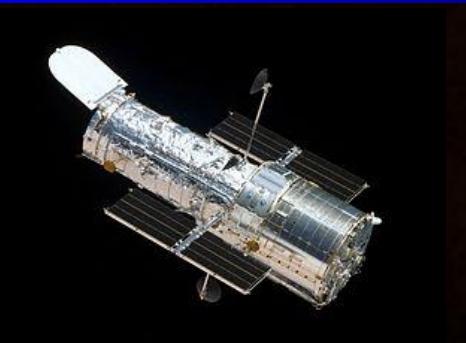
$^{36}\text{ArH}^+$

The results described in this article are reported in "**Detection of a Noble Gas Molecular Ion,  $^{36}\text{ArH}^+$ , in the Crab Nebula**", by M. J. Barlow et al., published in Science, 342, 6163, 1343-1345, 13 December 2013. DOI: 10.1126/science.124358213.

# ArH<sup>+</sup> ionty v Crab nebula

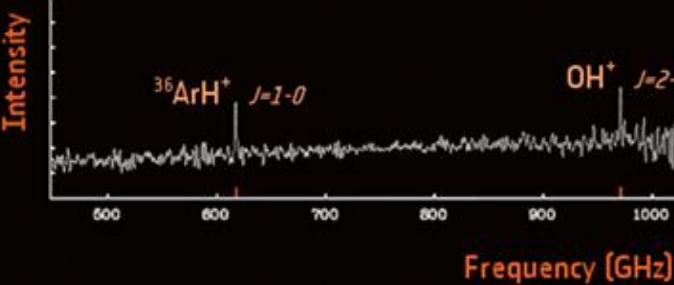
# Using ESA's Herschel Space Observatory

12 December 2013



$^{36}\text{ArH}^+$

$^{36}\text{ArH}^+$



$^{40}\text{Ar}$

The argon isotope found in the Crab Nebula is different from the one that dominates in Earth's atmosphere,  $^{40}\text{Ar}$ , which derives from the decay of a radioactive isotope of potassium ( $^{40}\text{K}$ ) present in our planet's rocks.

$^{36}\text{Ar}$

The Herschel data indicate that the argon hydride found in the Crab Nebula is made up of the argon isotope  $^{36}\text{Ar}$ . This is the first time that astronomers could identify the isotopic nature of an element in a supernova remnant.

"Finding that argon in the Crab Nebula consists of  $^{36}\text{Ar}$  was not surprising because this is the dominant isotope of argon across the Universe."

"And it's also the main argon isotope to be synthesised in the nuclear reactions during supernova explosions, so its detection in the Crab Nebula confirms that this iconic nebula was created by the explosive death of a massive star," explains Barlow.

## Astrophysical detection of the helium hydride ion $\text{HeH}^+$

Rolf Güsten<sup>1\*</sup>, Helmut Wiesemeyer<sup>1</sup>, David Neufeld<sup>2</sup>, Karl M. Menten<sup>1</sup>, Urs U. Graf<sup>3</sup>, Karl Jacobs<sup>3</sup>, Bernd Klein<sup>1,4</sup>, Oliver Ricken<sup>1</sup>, Christophe Risacher<sup>1,5</sup> & Jürgen Stutzki<sup>3</sup>

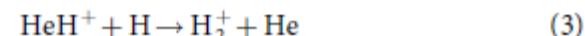
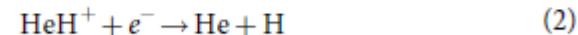
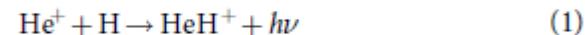
During the dawn of chemistry<sup>1,2</sup>, when the temperature of the young Universe had fallen below some 4,000 kelvin, the ions of the light elements produced in Big Bang nucleosynthesis recombined in reverse order of their ionization potential. With their higher ionization potentials, the helium ions  $\text{He}^{2+}$  and  $\text{He}^+$  were the first to combine with free electrons, forming the first neutral atoms; the recombination of hydrogen followed. In this metal-free and low-density environment, neutral helium atoms formed the Universe's first molecular bond in the helium hydride ion  $\text{HeH}^+$  through radiative association with protons. As recombination progressed, the destruction of  $\text{HeH}^+$  created a path to the formation of molecular hydrogen. Despite its unquestioned importance in the evolution of the early Universe, the  $\text{HeH}^+$  ion has so far eluded unequivocal detection in interstellar space. In the laboratory the ion was discovered<sup>3</sup> as long ago as 1925, but only in the late 1970s was the possibility that  $\text{HeH}^+$  might exist in local astrophysical plasmas discussed<sup>4–7</sup>. In particular, the conditions in planetary nebulae were shown to be suitable for producing potentially detectable column densities of  $\text{HeH}^+$ . Here we report observations, based on advances in terahertz spectroscopy<sup>8,9</sup> and a high-altitude observatory<sup>10</sup>, of the rotational ground-state transition of  $\text{HeH}^+$  at a wavelength of 149.1 micrometres in the planetary nebula NGC 7027. This confirmation of the existence of  $\text{HeH}^+$  in nearby interstellar space constrains our understanding of the chemical networks that control the formation of this molecular ion, in particular the rates of radiative association and dissociative recombination.

The deployment of the German Receiver for Astronomy at Terahertz Frequencies (GREAT)<sup>9</sup> heterodyne spectrometer on board the Stratospheric Observatory for Infrared Astronomy (SOFIA)<sup>10</sup> has now opened up new opportunities. Although the  $\text{HeH}^+ J = 1-0$  transition at  $149.137 \mu\text{m}$  (2010.183873 GHz; ref. <sup>21</sup>) cannot be observed from ground-based observatories, skies become transparent during high-altitude flights with SOFIA. The latest advances in terahertz technologies have



SOFIA

We then computed the equilibrium abundance of  $\text{HeH}^+$ , including the three reactions identified as being important in the layers in which  $\text{HeH}^+$  is most abundant<sup>7,13</sup>:



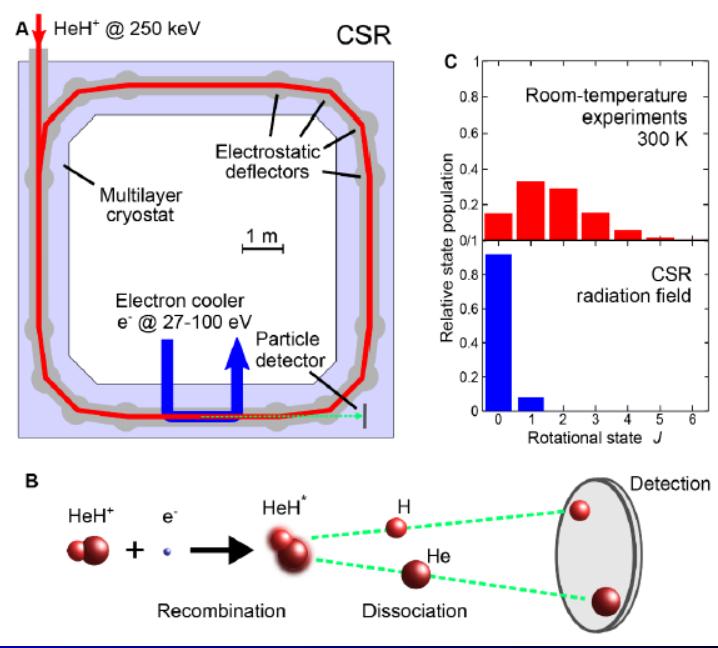
Cite as: O. Novotný *et al.*, *Science* 10.1126/science.aax5921 (2019).

## Quantum-state-selective electron recombination studies suggest enhanced abundance of primordial $\text{HeH}^+$

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## Dissociative Recombination of Cold $\text{HeH}^+$ Ions

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# 2018 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules

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**Table 1**  
Commonly Used Facility Abbreviations

Abbreviation	Description
ALMA	Atacama Large Millimeter/submillimeter Array
APEX	Atacama Pathfinder Experiment
ARO	Arizona Radio Observatory
ATCA	Australian Telescope Compact Array
BIMA	Berkeley-Illinois-Maryland Array
CSO	Caltech Submillimeter Observatory
FCRAO	Five College Radio Astronomy Observatory
FUSE	<i>Far Ultraviolet Spectroscopic Explorer</i>
GBT	Green Bank Telescope
IRAM	Institut de Radioastronomie Millimétrique
IRTF	Infrared Radio Telescope Facility
ISO	<i>Infrared Space Observatory</i>
KPNO	Kitt Peak National Observatory
MWO	Millimeter-wave Observatory
NRAO	National Radio Astronomy Observatory
OVRO	Owens Valley Radio Observatory
PdBI	Plateau de Bure Interferometer
SEST	Swedish-ESO Submillimeter Telescope
SMA	Sub-millimeter Array
SMT	Sub-millimeter Telescope
SOFIA	<i>Stratospheric Observatory for Infrared Astronomy</i>
UKIRT	United Kingdom Infrared Telescope

## 3. Known Interstellar Molecules

### Two-atom Molecules

#### 3.1. CH (*Methylidyne*)

Swings & Rosenfeld (1937) suggested that an observed line at  $\lambda = 4300 \text{ \AA}$  by Dunham (1937) using the Mount Wilson Observatory in diffuse gas toward a number of supergiant B stars might have been due to the  $^2\Delta \leftarrow ^2\Pi$  transition of CH, reported in the laboratory by Jevons (1932). McKellar (1940) later identified several additional transitions in observational data. The first radio identification was reported by Rydbeck et al. (1973) at 3335 MHz with the Onsala telescope toward more than a dozen sources using estimated fundamental rotational transition frequencies from Shklovskii (1953), Goss (1966), and Baird & Bredohl (1971). The first direct

measurement of the CH rotational spectrum was reported by Brazier & Brown (1983).

#### 3.64. $H_3^+$

First suggested as a possible interstellar molecule in Martin et al. (1961),  $H_3^+$  was detected 35 years later in absorption toward GL 2136 and W33A by Geballe & Oka (1996) using UKIRT to observe three transitions of the  $\nu_2$  fundamental band near  $3.7 \mu\text{m}$ . The laboratory work was performed by Oka (1980).

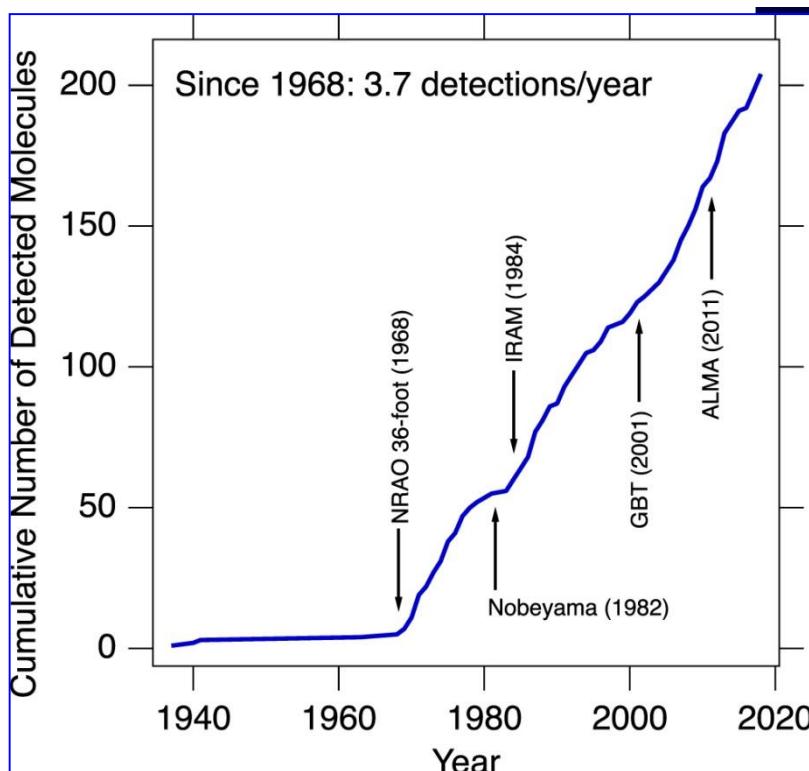
# Molecules in interstellar space

Not actualized, approximation

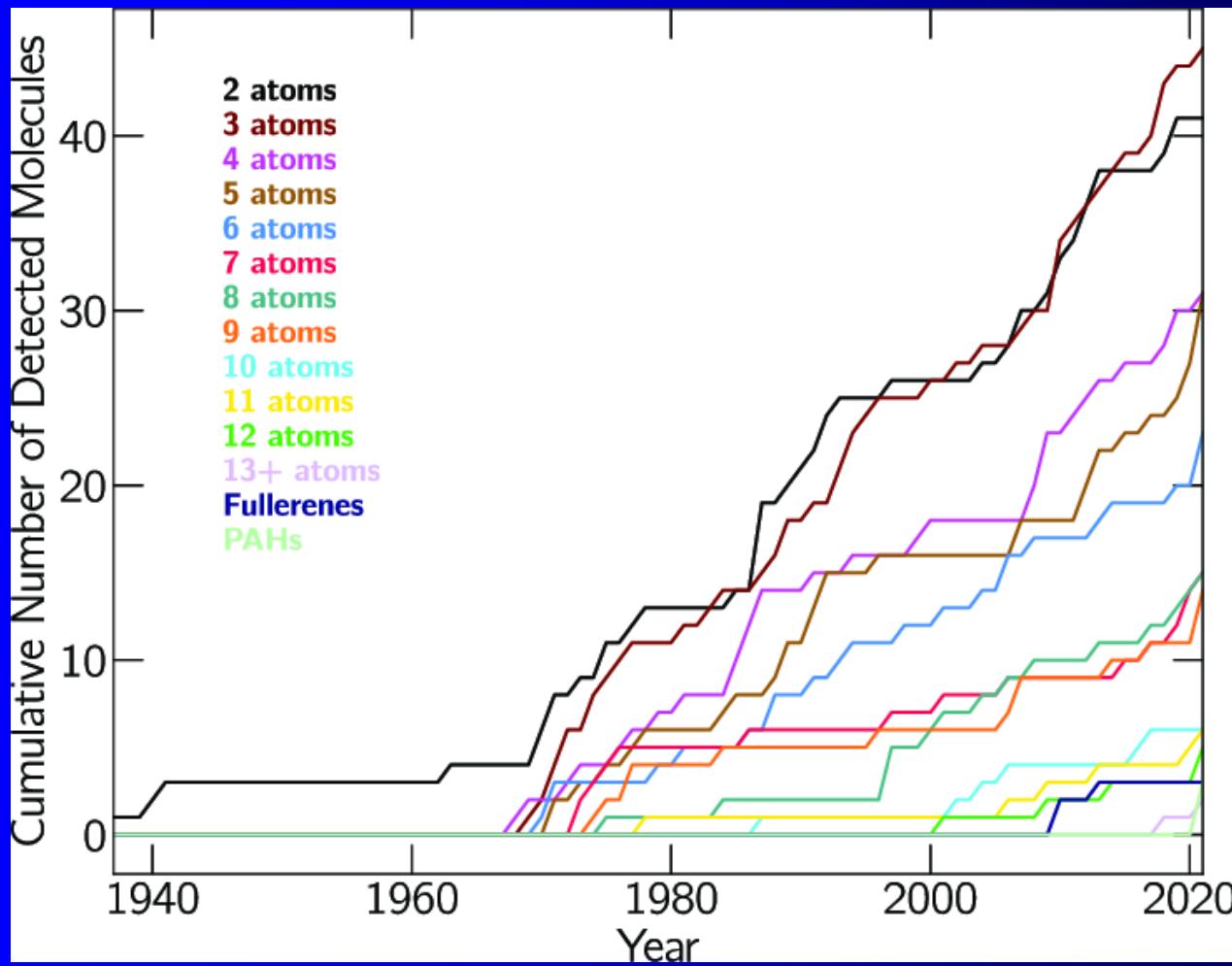
	3	4	5	6	7	8	9	10	11	13
H <sub>2</sub>	C <sub>3</sub>	c-C <sub>3</sub> H	C <sub>5</sub>	C <sub>5</sub> H	C <sub>6</sub> H	CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> C <sub>4</sub> H	CH <sub>3</sub> C <sub>5</sub> N?	HC <sub>9</sub> N	HC <sub>11</sub> N
AlF	C <sub>2</sub> H	l-C <sub>3</sub> H	C <sub>4</sub> H	l-H <sub>2</sub> C <sub>4</sub>	CH <sub>2</sub> CHCN	HCOOCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>3</sub> ) <sub>2</sub> CO		
AlCl	C <sub>2</sub> O	C <sub>3</sub> N	C <sub>4</sub> Si	C <sub>2</sub> H <sub>4</sub>	CH <sub>3</sub> C <sub>2</sub> H	CH <sub>3</sub> COOH?	(CH <sub>3</sub> ) <sub>2</sub> O	NH <sub>2</sub> CH <sub>2</sub> COOH?		
C <sub>2</sub>	C <sub>2</sub> S	C <sub>3</sub> O	l-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> CN	HC <sub>5</sub> N	C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH			
CH	CH <sub>2</sub>	C <sub>3</sub> S	c-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> NC	HCOCH <sub>3</sub>	H <sub>2</sub> C <sub>6</sub>	HC <sub>7</sub> N			
<b>CH<sup>+</sup></b>	HCN	C <sub>2</sub> H <sub>2</sub>	CH <sub>2</sub> CN	CH <sub>3</sub> OH	NH <sub>2</sub> CH <sub>3</sub>	CH <sub>2</sub> OHCHO	C <sub>8</sub> H			
CN	HCO	<b>CH<sub>2</sub>D<sup>+</sup>?</b>	CH <sub>4</sub>	CH <sub>3</sub> SH	c-C <sub>2</sub> H <sub>4</sub> O					
CO	<b>HCO<sup>+</sup></b>	HCCN	HC <sub>3</sub> N	<b>HC<sub>3</sub>NH<sup>+</sup></b>	CH <sub>2</sub> CHOH					
<b>CO<sup>+</sup></b>	<b>HCS<sup>+</sup></b>	<b>HCNH<sup>+</sup></b>	HC <sub>2</sub> NC	HC <sub>2</sub> CHO						
CP	<b>HOC<sup>+</sup></b>	HNCO	HCOOH	NH <sub>2</sub> CHO						
CSi	H <sub>2</sub> O	HNCS	H <sub>2</sub> CHN	C <sub>5</sub> N						
HCl	H <sub>2</sub> S	<b>HOCO<sup>+</sup></b>	H <sub>2</sub> C <sub>2</sub> O							
KCl	HNC	H <sub>2</sub> CO	H <sub>2</sub> NCN							
NH	HNO	H <sub>2</sub> CN	HNC <sub>3</sub>							
NO	MgCN	H <sub>2</sub> CS	SiH <sub>4</sub>							
NS	MgNC	<b>H<sub>3</sub>O<sup>+</sup></b>	<b>H<sub>2</sub>COH<sup>+</sup></b>							
NaCl	<b>N<sub>2</sub>H<sup>+</sup></b>	NH <sub>3</sub>								
OH	N <sub>2</sub> O	SiC <sub>3</sub>								
PN	NaCN									
SO	OCS									
<b>SO<sup>+</sup></b>	SO <sub>2</sub>									
SiN	c-SiC <sub>2</sub>									
SiO	CO <sub>2</sub>									
SiS	NH <sub>2</sub>									
CS	<b>H<sub>3</sub><sup>+</sup></b>									
HF		SiCN								
SH		AINC								
FeO?										

~2015

16 JULY 2015 | VOL 523 | NATURE | 323



Cumulative number of known interstellar molecules over time.  
Commissioning dates of major contributing facilities are noted  
with arrows. [McGuire 2018]

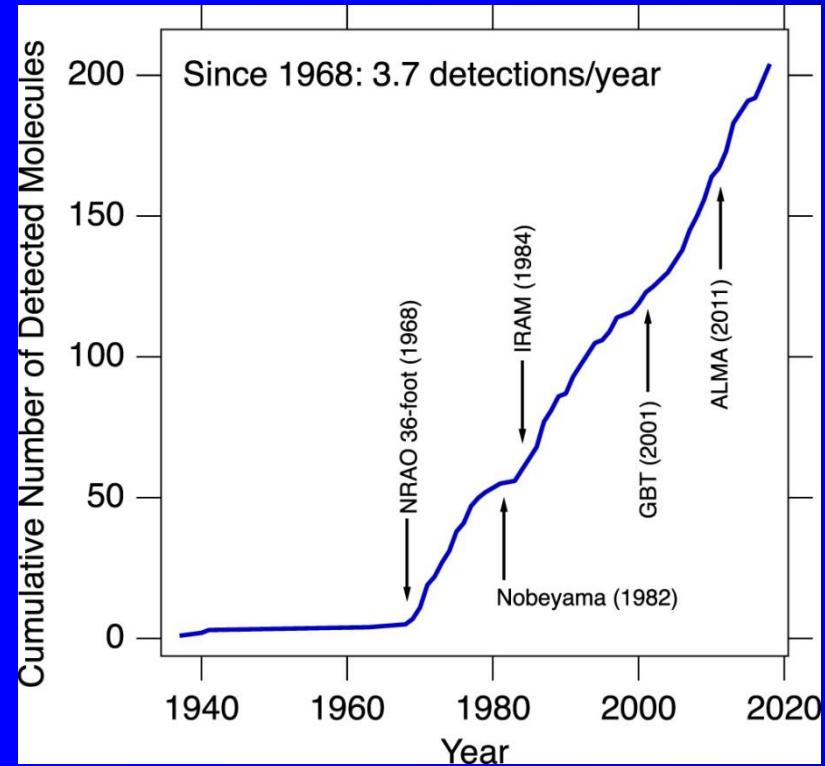


Cumulative number of known interstellar molecules with 2-13 atoms, as well as fullerene molecules, as a function of time. The traces are color coded by number of atoms and labeled on the right.

# Molecules in interstellar space

Not actualized, approximation

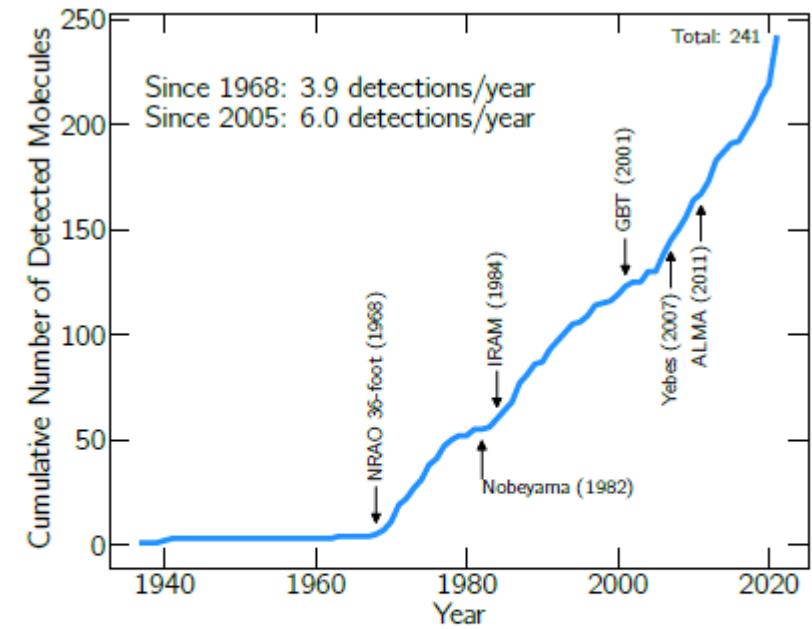
16 JULY 2015 | VOL 523 | NATURE | 323



Cumulative number of known interstellar molecules over time. Commissioning dates of major contributing facilities are noted with arrows. [McGuire 2018]

actualized, approximation

2021



**Figure 1.** Cumulative number of known interstellar molecules over time. After the birth of molecular radio astronomy in the 1960s, there have been on average 3.9 new detections per year. The commissioning dates of several major contributing facilities are noted with arrows.

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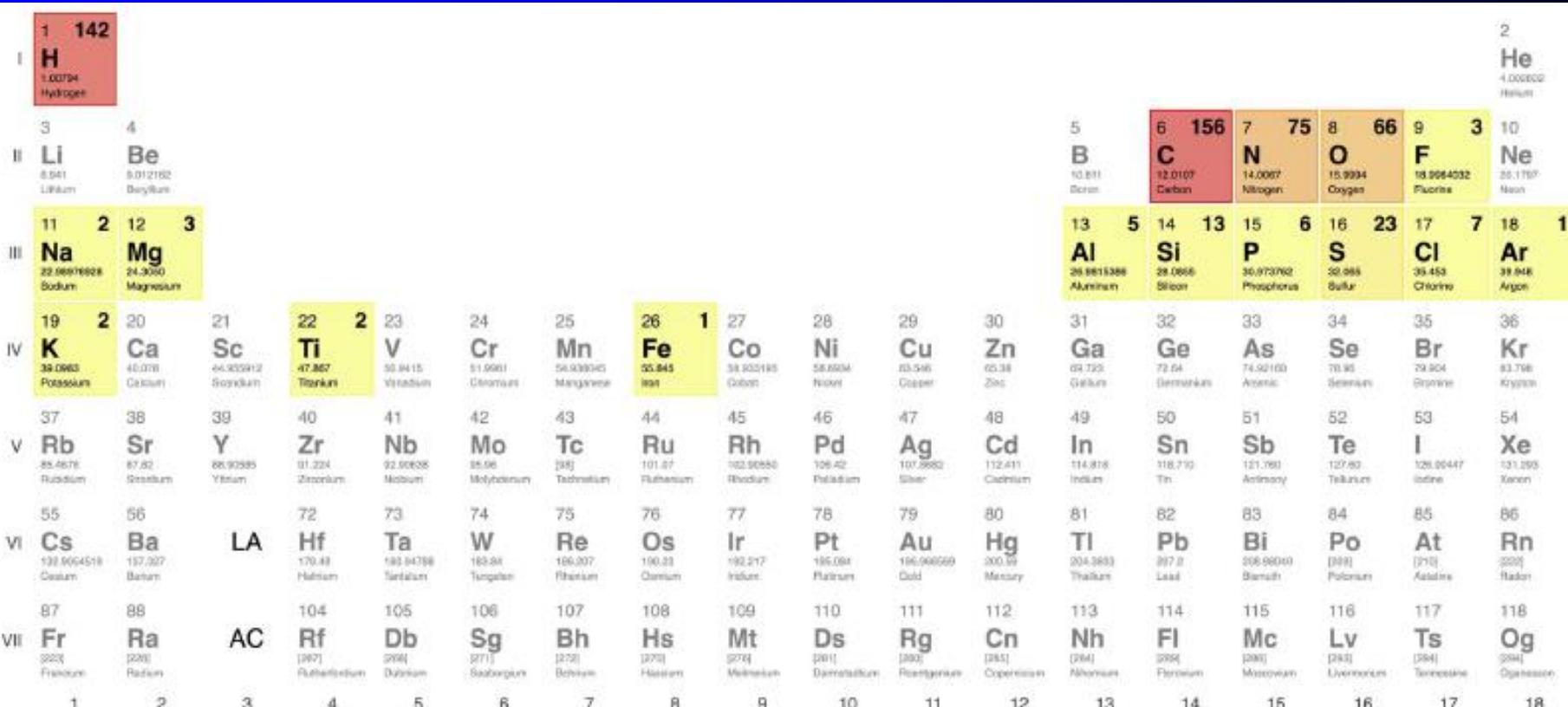
2021 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules

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**Figure 6.** Periodic table of the elements, absent the lanthanide and actinide series, color-coded by number of detected species containing each element. For those elements with detected ISM molecules, that number is displayed in the upper right of each cell.

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<https://doi.org/10.3847/1538-4365/aae5d2>

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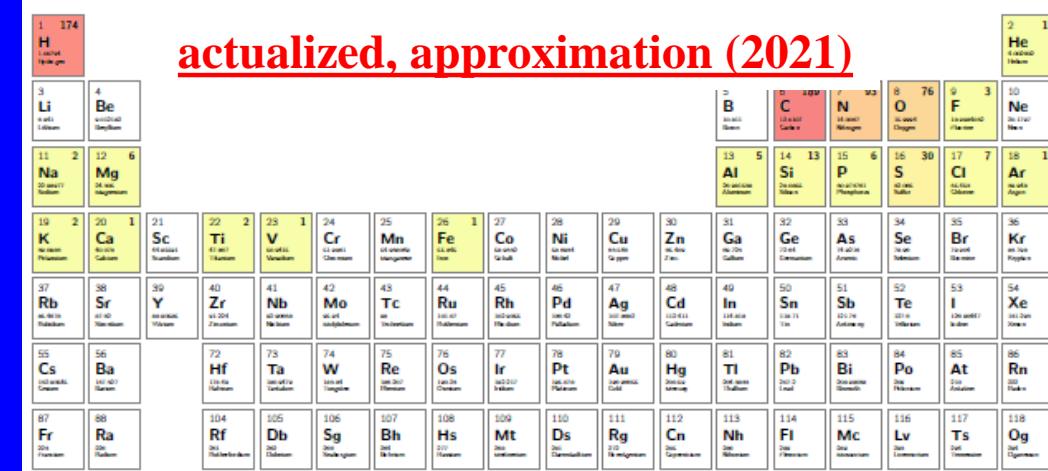
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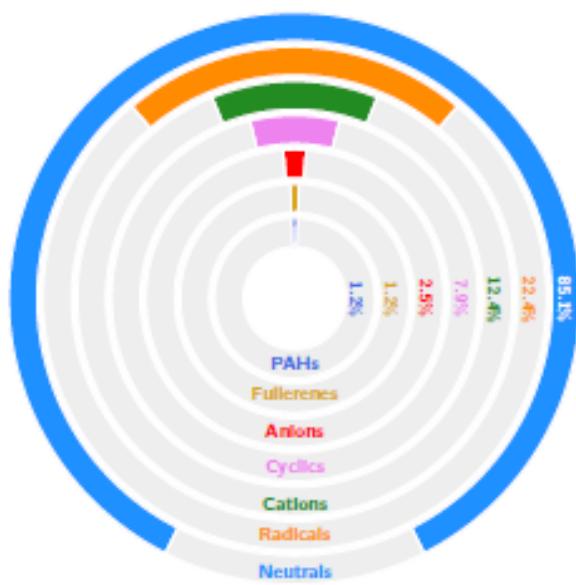
<sup>1</sup> National Radio Astronomy Observatory, Charlottesville, VA 22903, USA

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*Received 2018 May 27; revised 2018 September 20; accepted 2018 September 20; published 2018 November 26*



**Figure 6.** Periodic table of the elements, absent the lanthanide and actinide series, colored by number of detected species containing each element. For those elements with detected ISM molecules, that number is displayed in the upper right of each cell.



**Figure 10.** Percentage of known interstellar molecules that are neutral, cationic, anionic, radical species, or cyclic. Many molecules fall into more than one of these categories (e.g. most radical species have a net neutral charge).

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## 2021 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules

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# Interstellar medium

92.1% of nucleons in the universe are protons

7.8% are helium nuclei !

0.1%.....C,N,O,S,Si....

Cosmic abundance

H

He

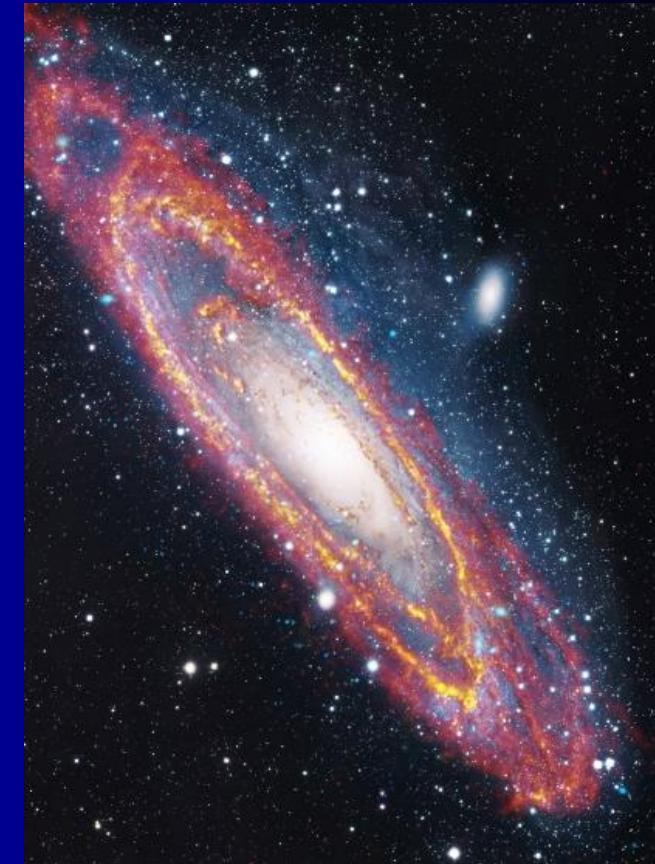
■ ■ ■ ■  
C N O Ne

Mg

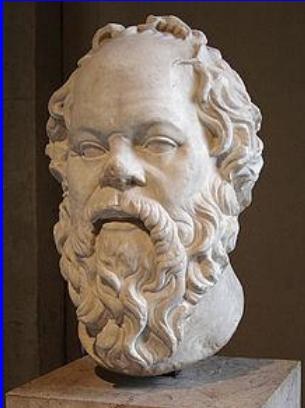
· · · ·  
Si S Ar

Fe

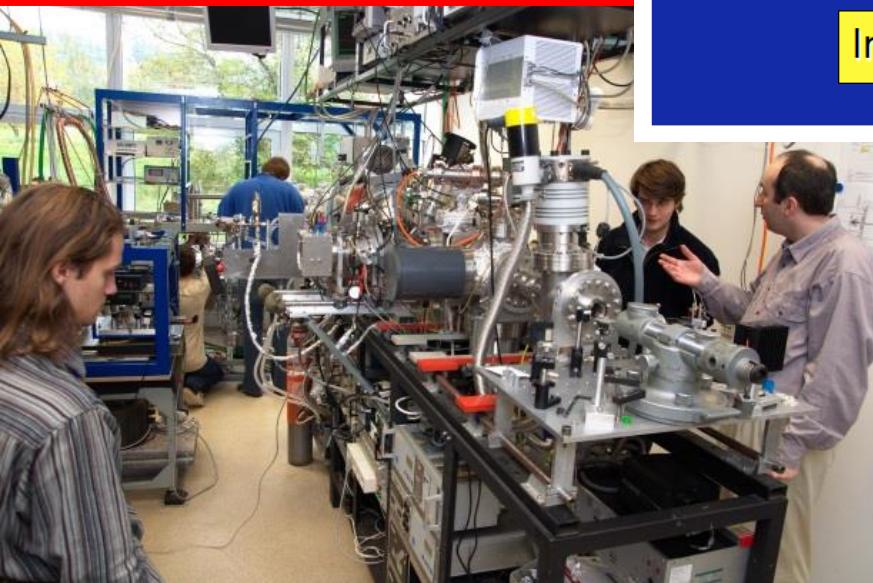
~0.005%.....D



Andromeda composite



Scio me nihil scire



# The astrochemistry game plan

Laboratory astrophysics and related theory

Spectroscopy

Collisional excitation rate coefficients

Bimolecular reaction rate coefficients

Grain surface reactions

Photoionization and photodissociation cross-sections

Observations of astrophysical molecules

Emission line luminosities

Absorption line optical depths

Astrochemical modeling of ...

Diffuse IS cloud

Dense IS clouds

Photodissociation regions

Circumstellar outflows

X-irradiated regions

Excitation and radiative transfer

Information of general astrophysical interest

Plasma physics laboratory

KFPP MFF UK



Načo chodit' do školy

2014

FIRST TIME-DEPENDENT STUDY OF H<sub>2</sub> AND H<sub>3</sub><sup>+</sup> ORTHO-PARA CHEMISTRY IN THE DIFFUSE INTERSTELLAR MEDIUM: OBSERVATIONS MEET THEORETICAL PREDICTIONS\*

T. ALBERTSSON<sup>1</sup>, N. INDRILO<sup>2</sup>, H. KRECKEL<sup>3</sup>, D. SEMENOV<sup>1</sup>, K. N. CRABTREE<sup>4</sup>, AND TH. HENNING<sup>1</sup>

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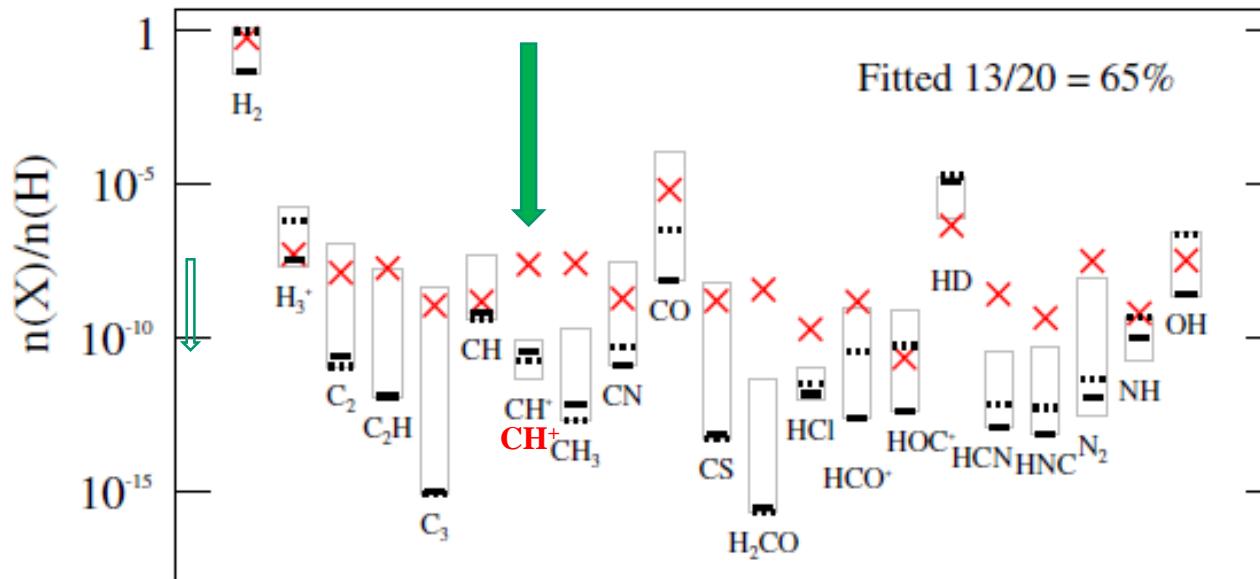
<sup>3</sup> Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany

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Received 2013 December 4; accepted 2014 March 28; published 2014 May 2

## The chemistry in the diffuse interstellar medium (ISM)

THE ASTROPHYSICAL JOURNAL, 787:44 (10pp), 2014 May 20



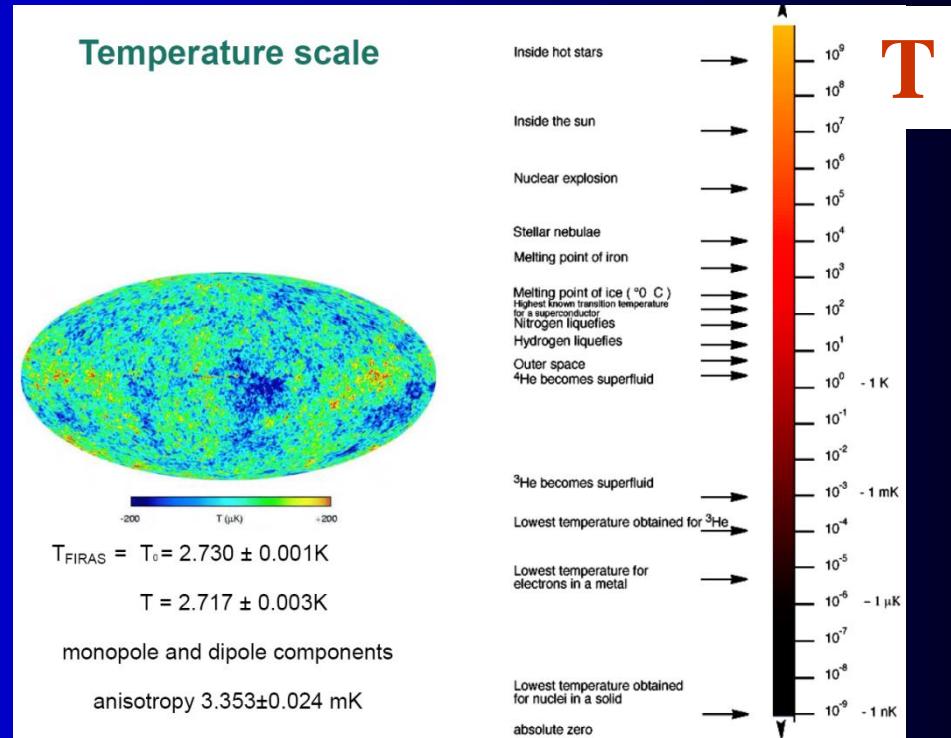
**Figure 6.** Comparison of observed abundances (red crosses) to modeled values of key species in diffuse clouds. Gray boxes show the range of abundances calculated from the considered models (Table 2) and black lines show abundances from the best-fit model “2X+C15” (30 K, solid line, and 90 K, dotted line).

(A color version of this figure is available in the online journal.)

# Temperature scale should be logarithmic

## Far Infrared Absolute Spectrophotometer (FIRAS)

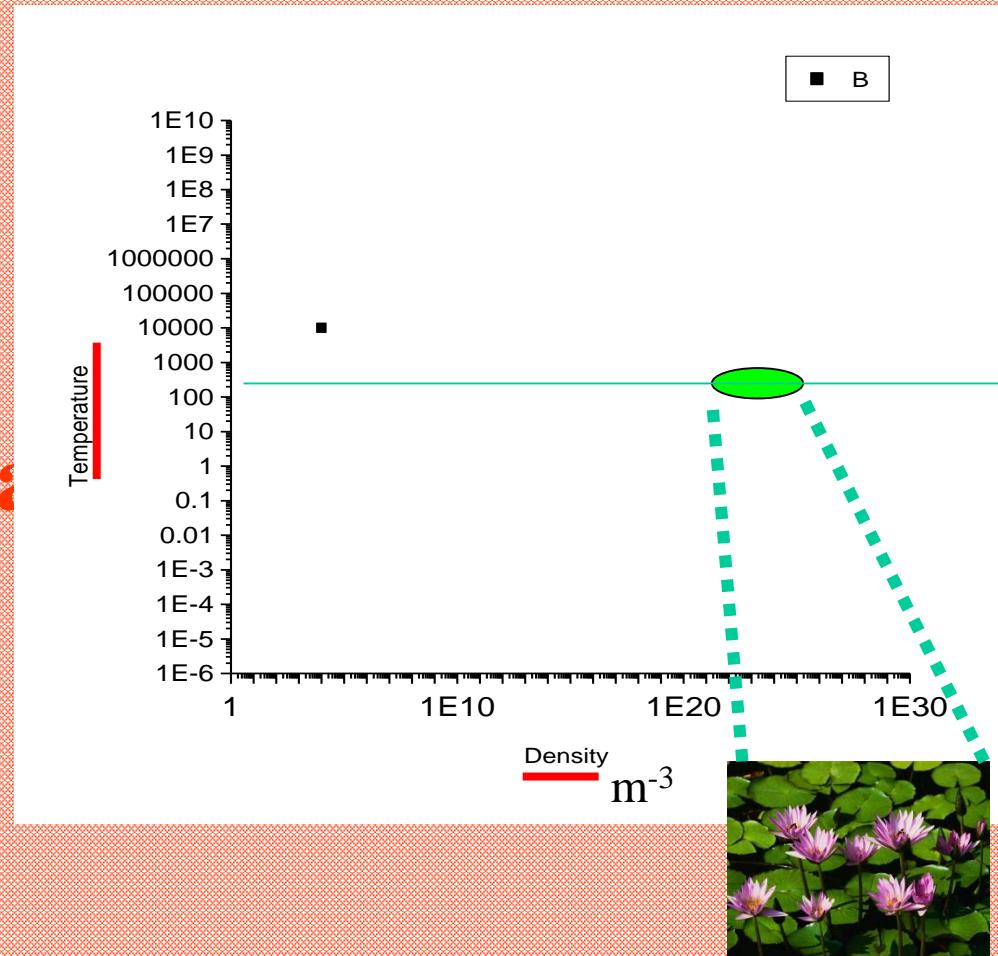
cosmic microwave background



The **cosmic microwave background (CMB, CMBR)**, Big Bang cosmology, is electromagnetic radiation which is a remnant from an early stage of the universe, also known as "relic radiation". The CMB is faint cosmic background radiation filling all space. It is an important source of data on the early universe because it is the oldest electromagnetic radiation in the universe, dating to the epoch of recombination. With a traditional optical telescope, the space between stars and galaxies (the *background*) is completely dark. However, a sufficiently sensitive radio telescope shows a faint background noise, or glow, almost isotropic, that is not associated with any star, galaxy, or other object. This glow is strongest in the microwave region of the radio spectrum. The accidental discovery of the CMB in 1965 by American radio astronomers Arno Penzias and Robert Wilson<sup>[1][2]</sup> was the culmination of work initiated in the 1940s, and earned the discoverers the 1978 Nobel Prize in Physics.

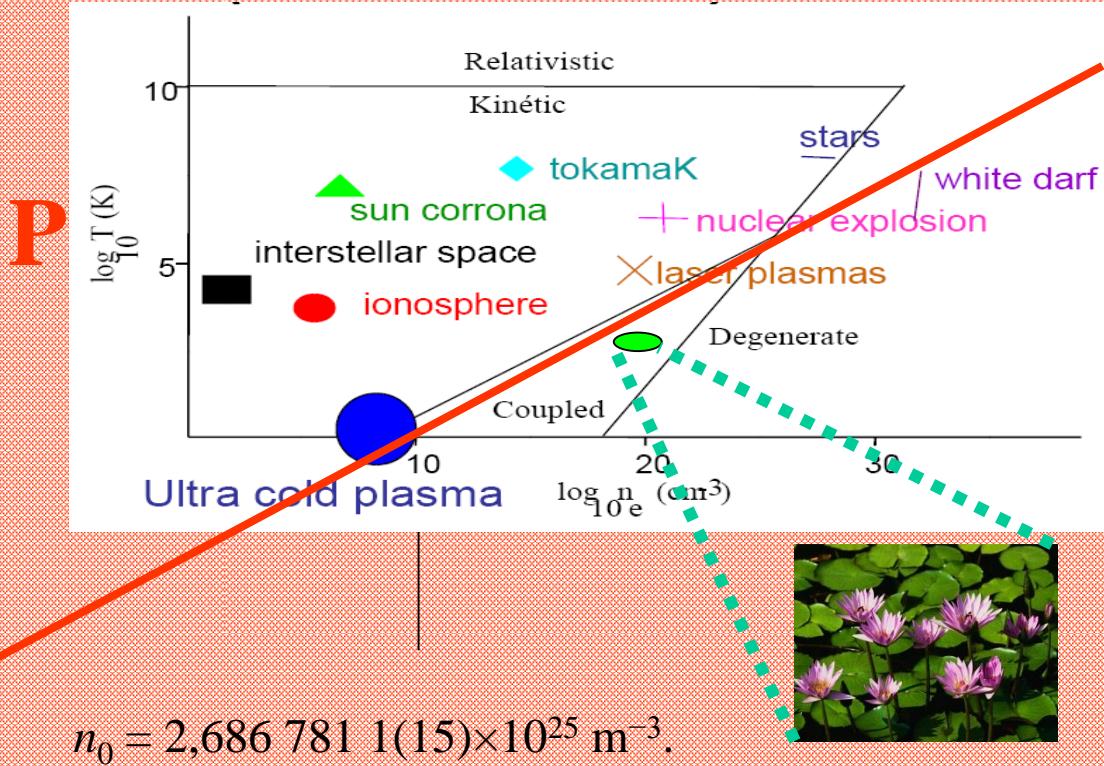
# Plasma

Pla



## Not actualized, approximation

Plazma .... $n_e$  ... $T_e$  .... T



$$W_{kin} \sim W_{Pot.elektrost}$$

$$\frac{3}{2} kT \sim \frac{e^2}{\varepsilon a} \sim \frac{e^2}{\varepsilon N^{-1/3}}$$

$$T \sim \frac{10^{-38}}{k\varepsilon} N^{1/3}$$

$$T_K = 1K \Rightarrow N_K = 10^9 \text{ m}^{-3}$$

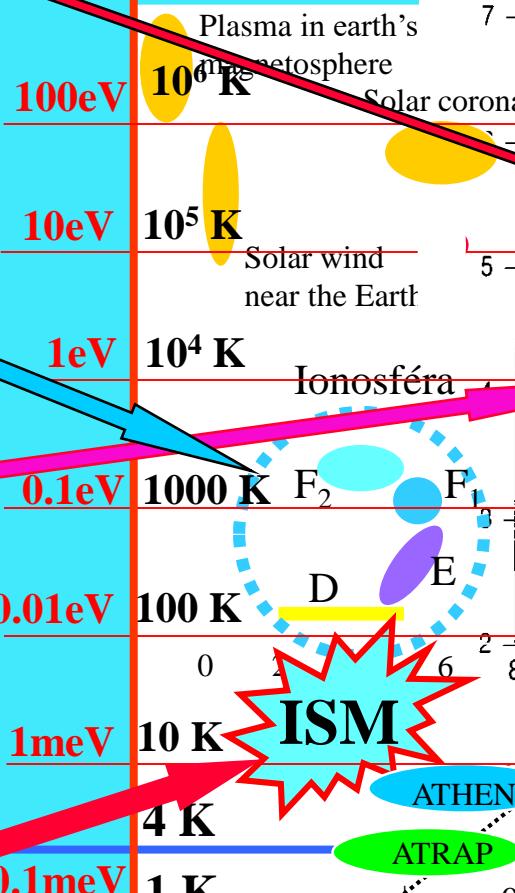
# Temperatures and energies



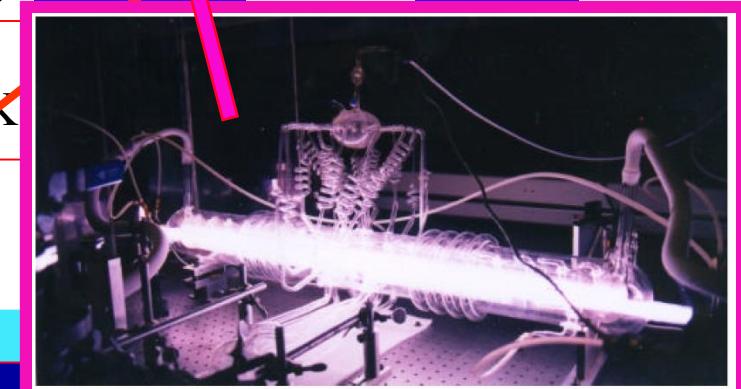
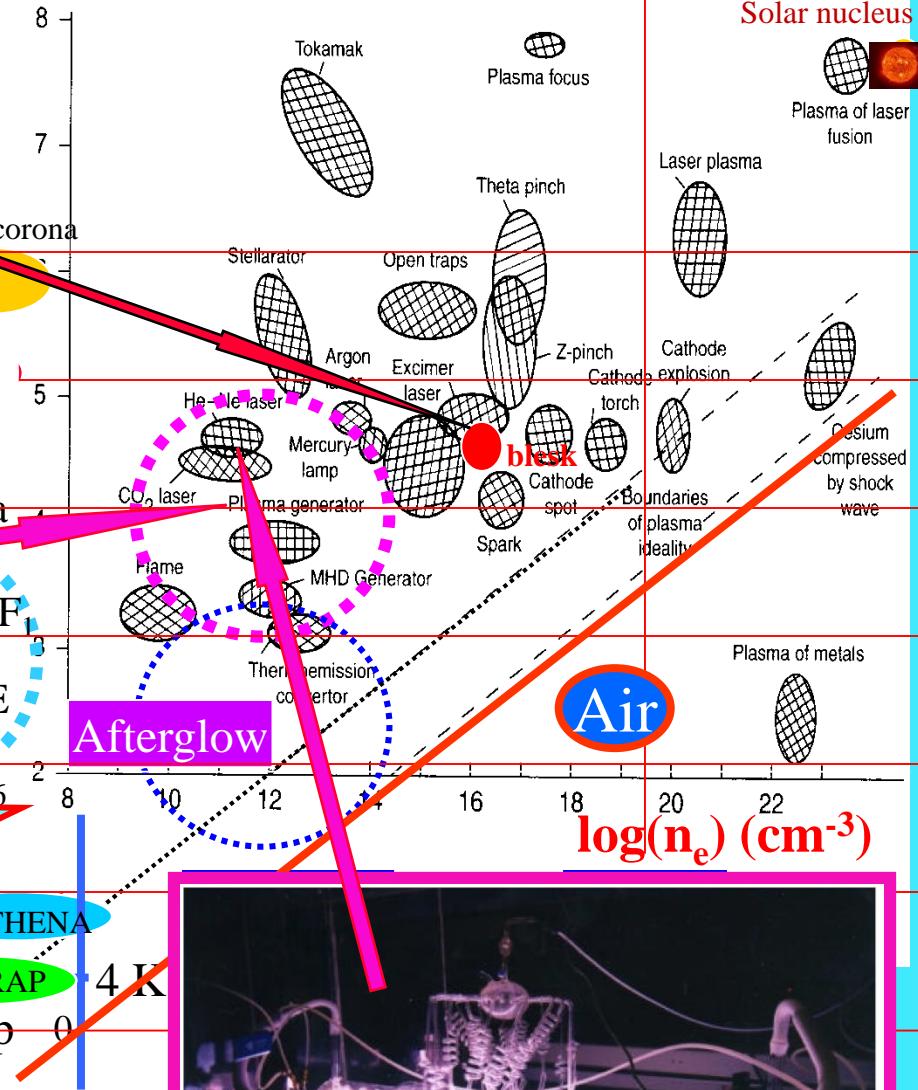
$$E \leftrightarrow kT$$

$$1\text{eV} \sim 11\,604.505 \text{ K}$$

$$1\text{K} \sim 9 \times 10^{-5} \text{ eV}$$



$\log T_e (\text{K})$



PLASMA AS A STATE OF MATTER

Solar nucleus  
Plasma of laser fusion

Not actualized, approximation

# Parameters of laboratory plasmas

Not actualized, approximation

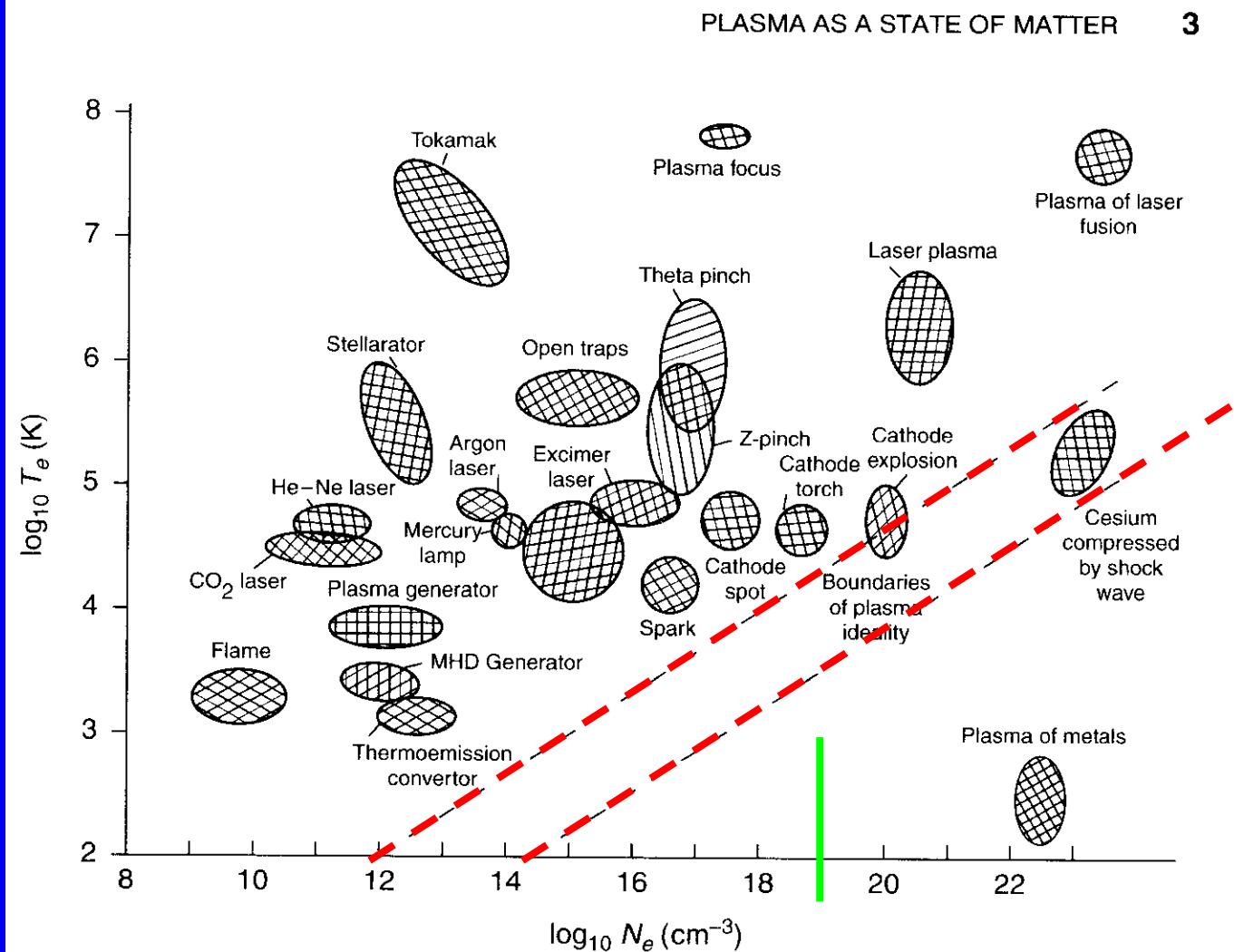
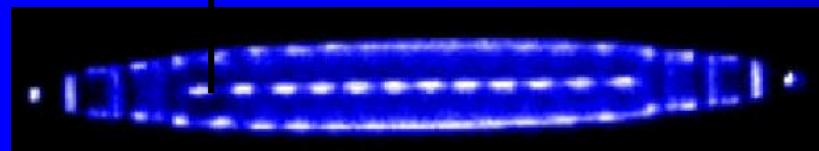
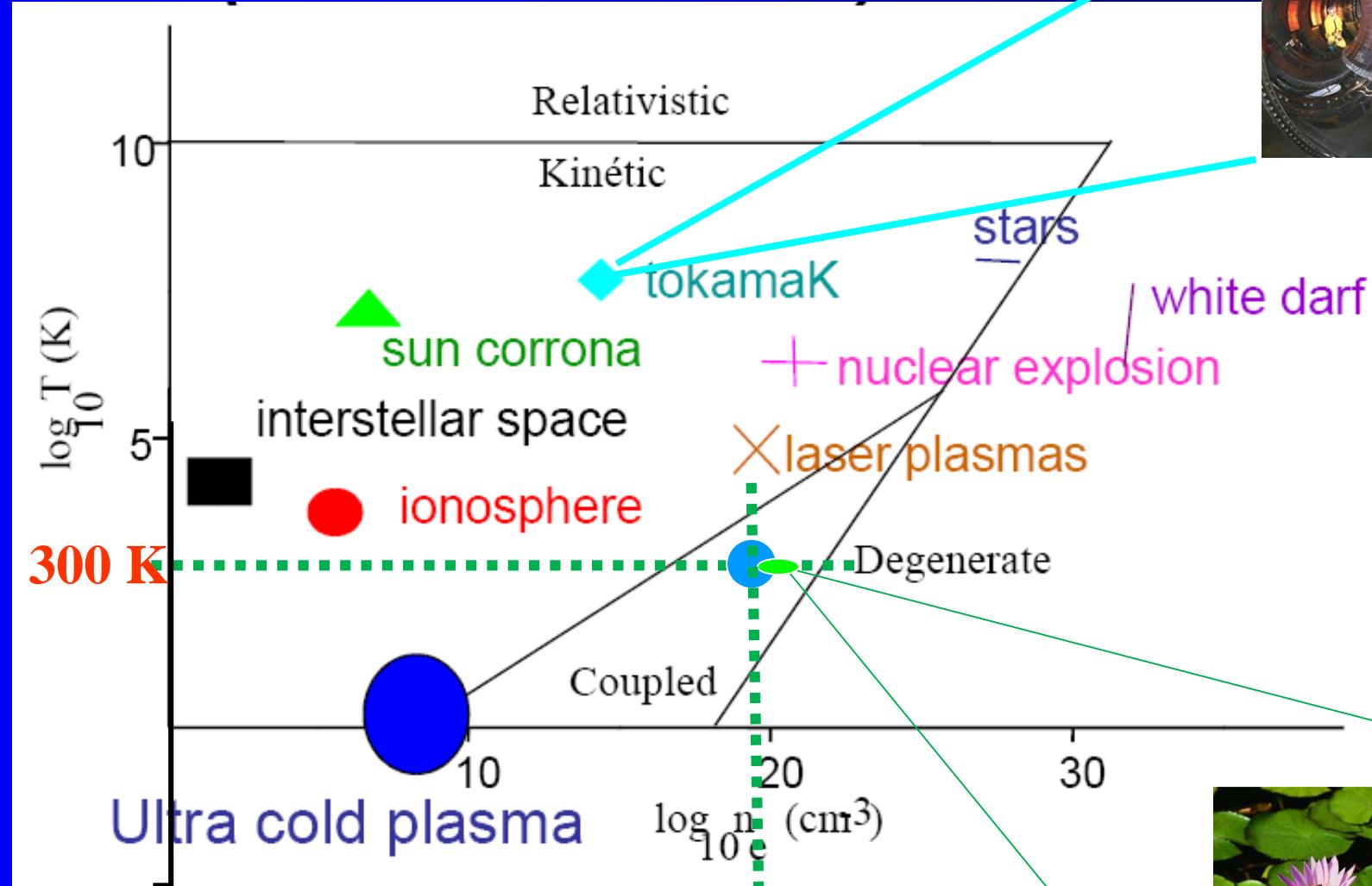
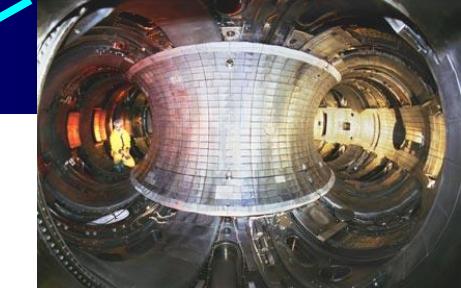


Figure 1.1 Parameters of laboratory plasmas.

# Electron temperature and electron number density - PLASMA



Experiment:  $T \sim 6 \text{ mK}$



# Parameters of plasmas found in nature

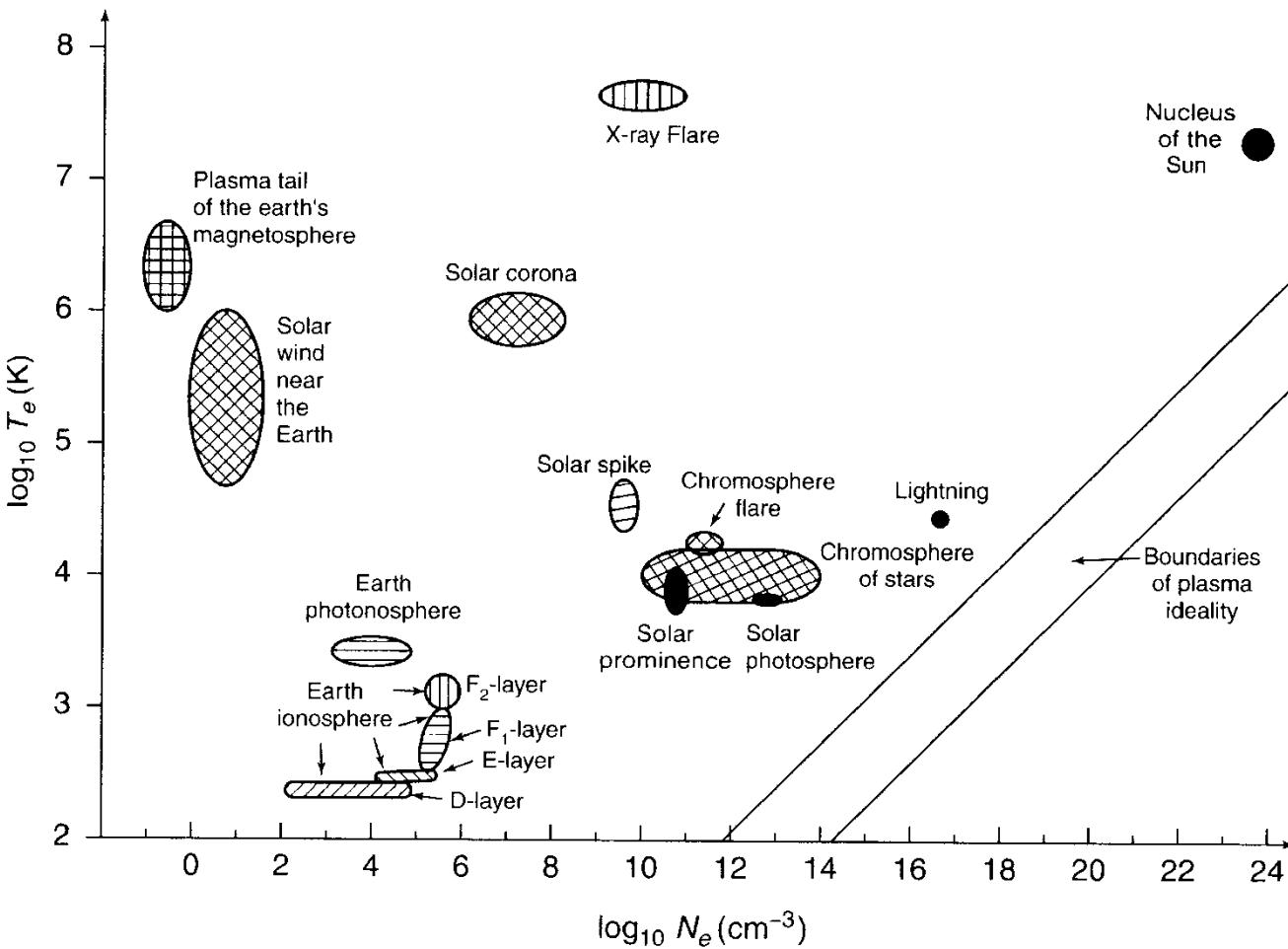


Figure 1.2 Parameters of plasmas found in nature.

# Electron and gas temperatures in plasmas

4 PLASMA IN NATURE AND IN LABORATORY SYSTEMS

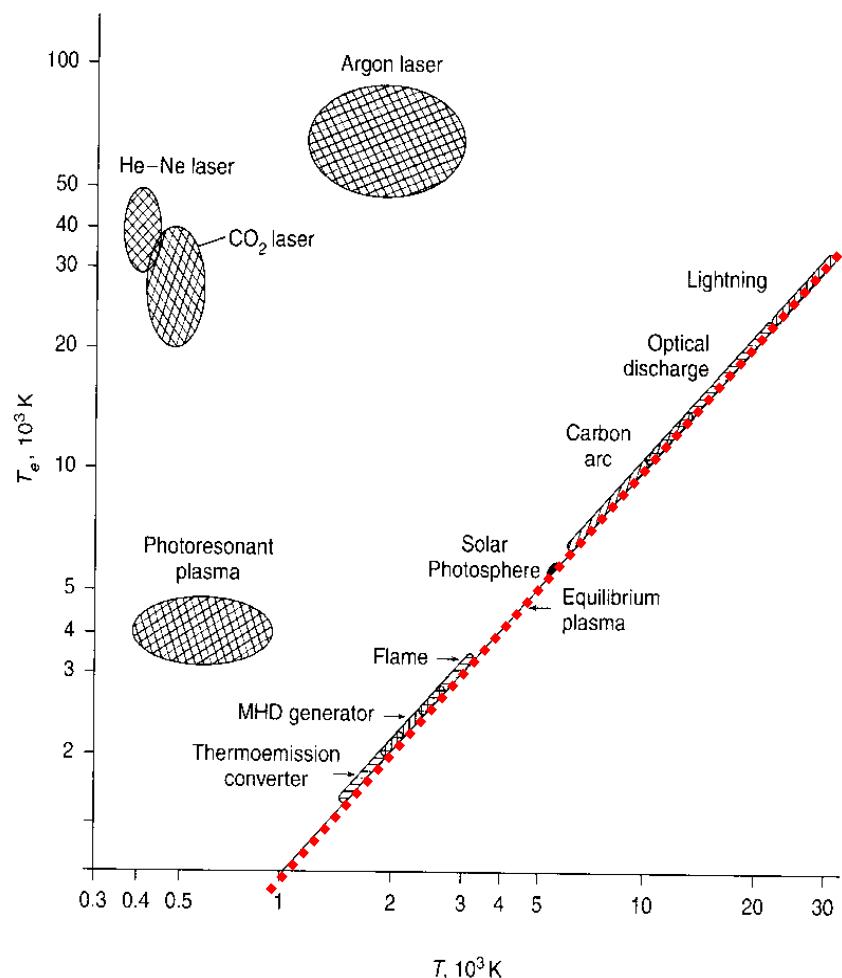


Figure 1.3 Electron and gas temperatures of laboratory plasmas. The straight line corresponds to the equilibrium plasma whose electron and gas temperatures are the same.

Difference in electron, ion and neutral gas temperature in plasma

Equilibrium; relaxation time,

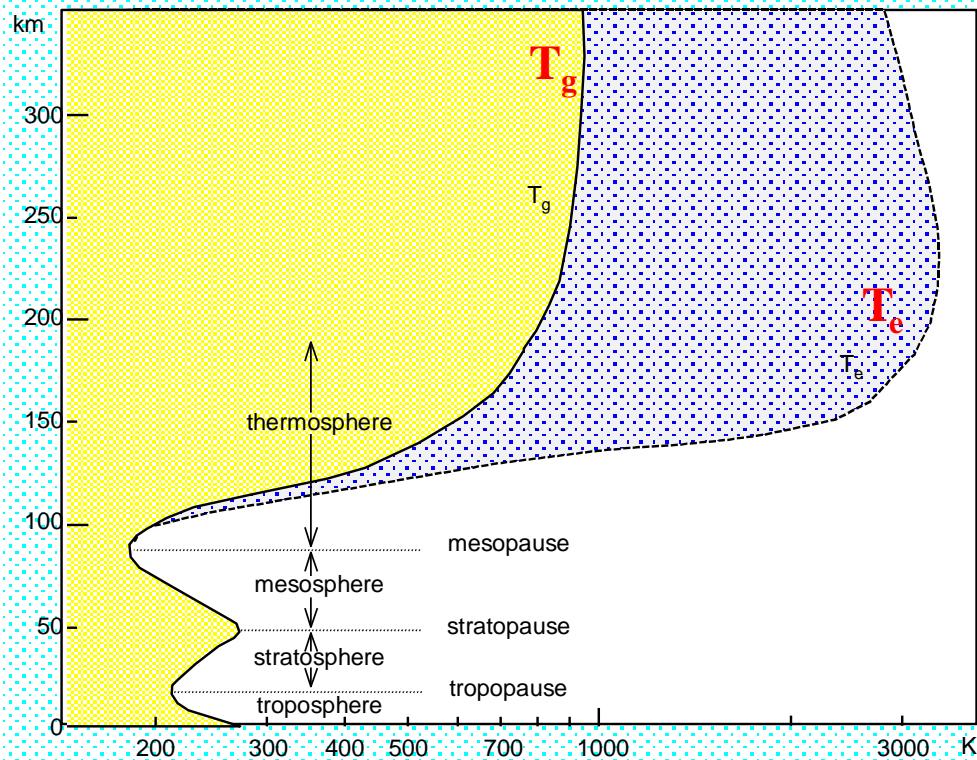
Probability of interactions...

Collisional frequency, Energy transfer

cross section

# Temperature in the ionosphere

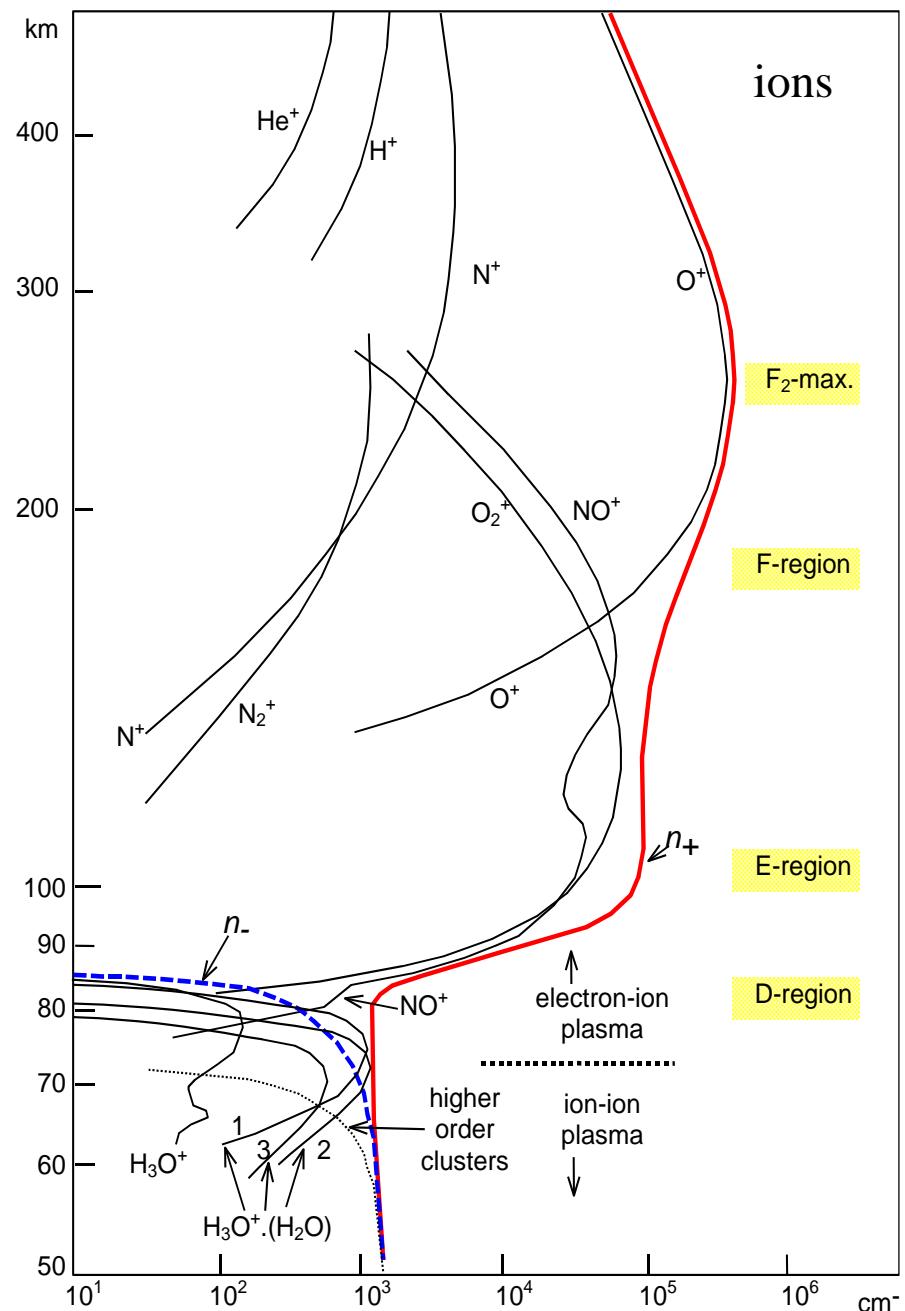
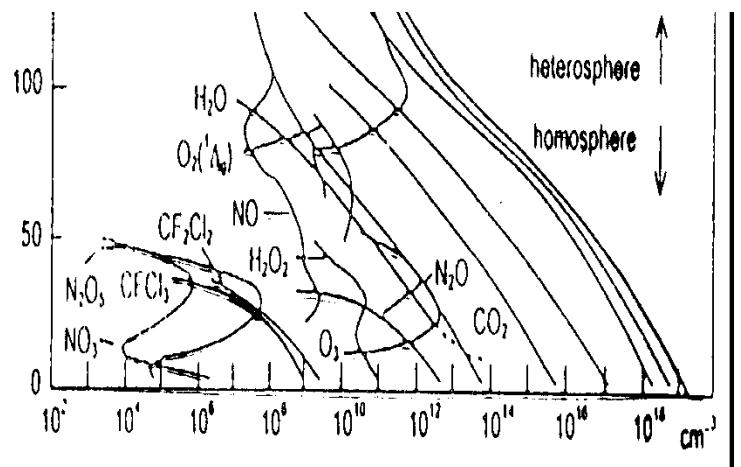
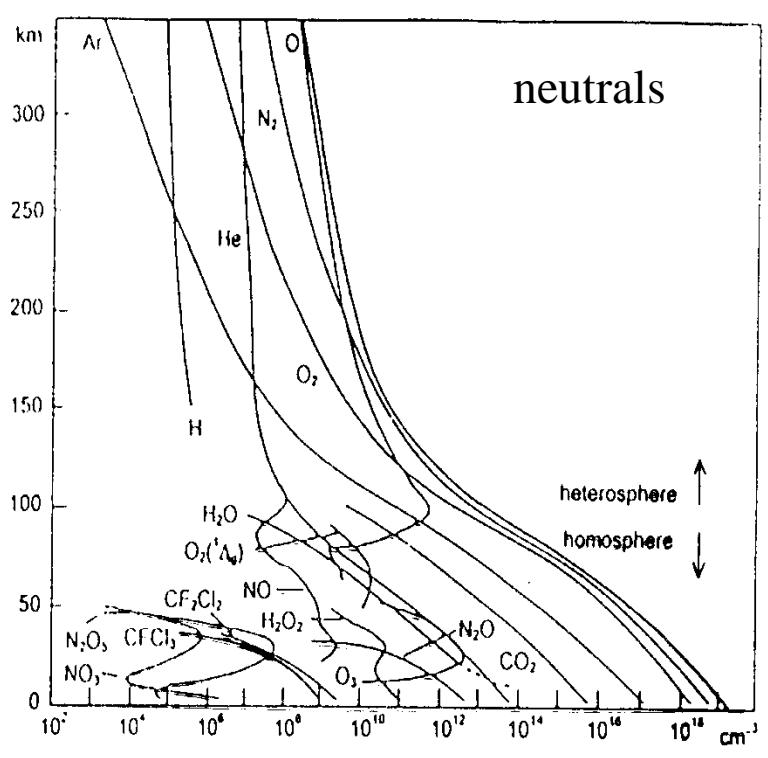
## Temperatures in the ionosphere



# Ions chemistry

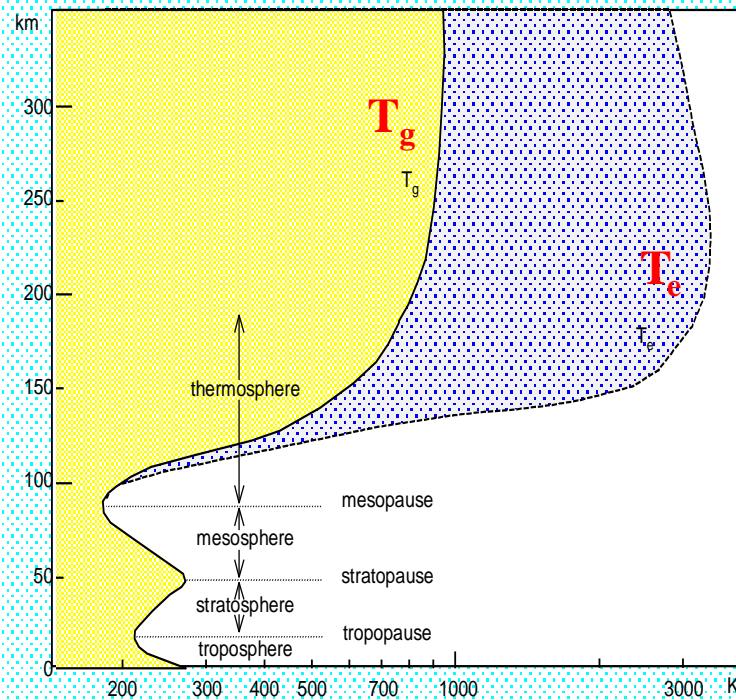
$$n_0 = 2,686\,781\,1(15) \times 10^{19} \text{ cm}^{-3}$$

# Ions in the terrestrial atmosphere

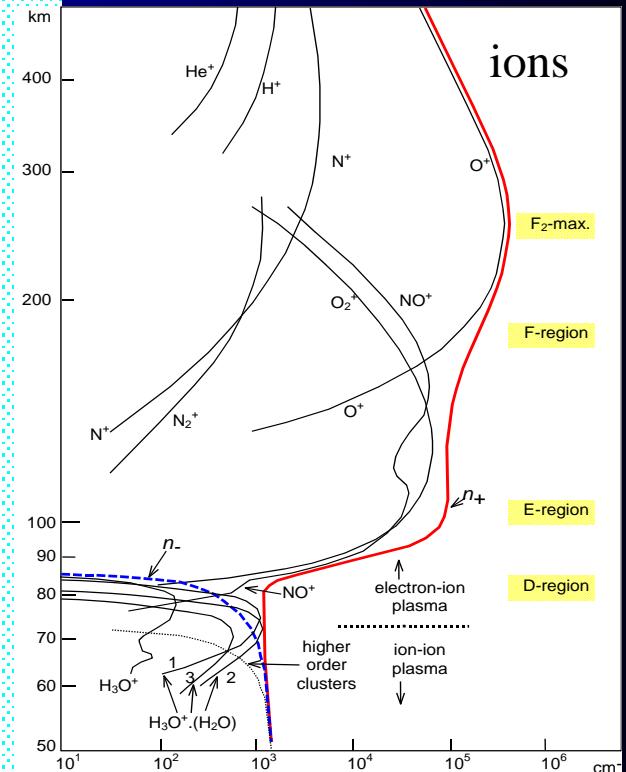


# Ions in the terrestrial atmosphere

## Temperatures in the ionosphere



Recombination??  $\alpha(T)$



# Crab Nebula

ISM

Hydrogen only??

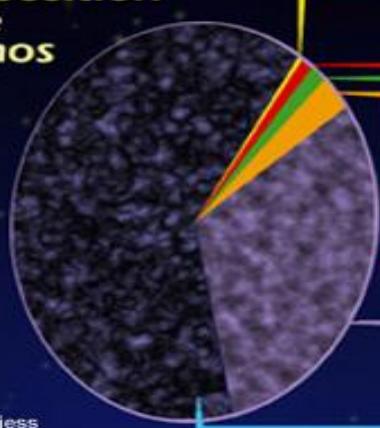
Ions chemistry

Electron – ion interactions

Negative ions ??

..... ??

## Composition of the Cosmos



NASA/A. Riess

Heavy  
elements:  
0.03%

Ghostly  
neutrinos:  
0.3%

Stars:  
0.5%

Free hydrogen  
and helium:  
4%

Dark  
matter:  
30%

Dark  
energy:  
65%

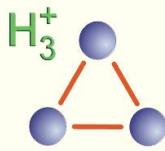
Scio me nihil scire

Hubble  
Heritage

SA and The Hubble Heritage Team (STScI/AURA)

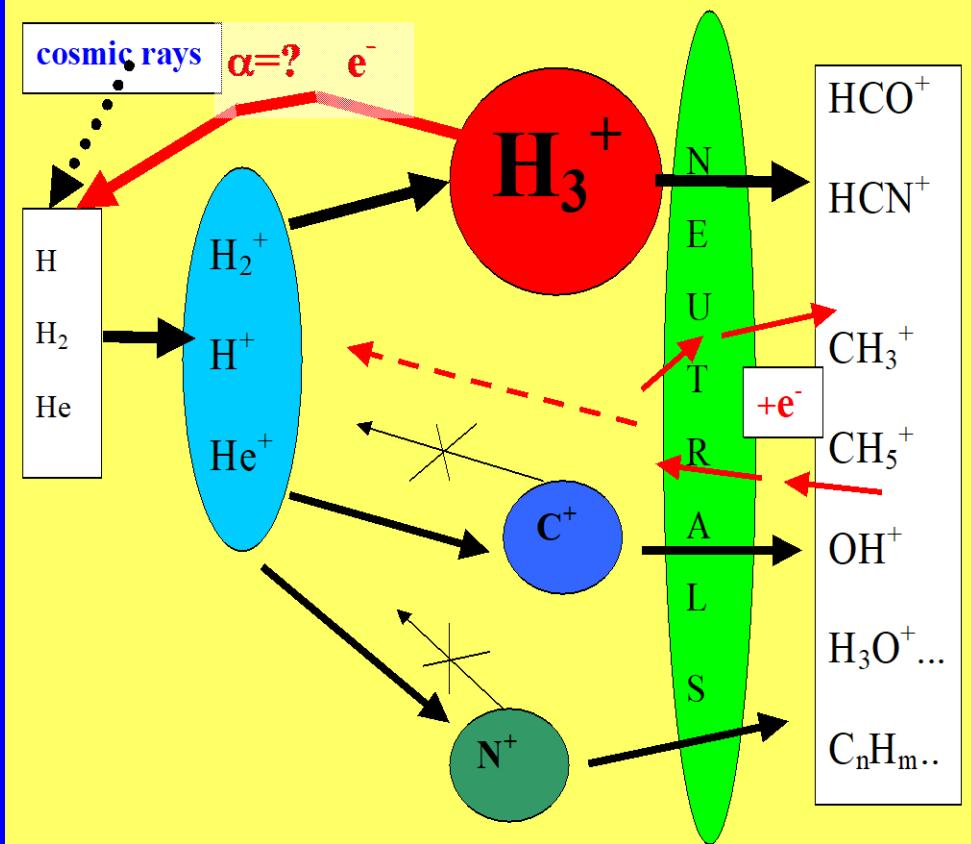
# Interstellar medium

92.1% of nucleons in the universe are protons  
7.8% are helium nuclei !



Hydrogen only??

## DENSE INTERSTELLAR CLOUDS



$\alpha=?$   
T ~ 10-50K



# Interstellar medium, HD role

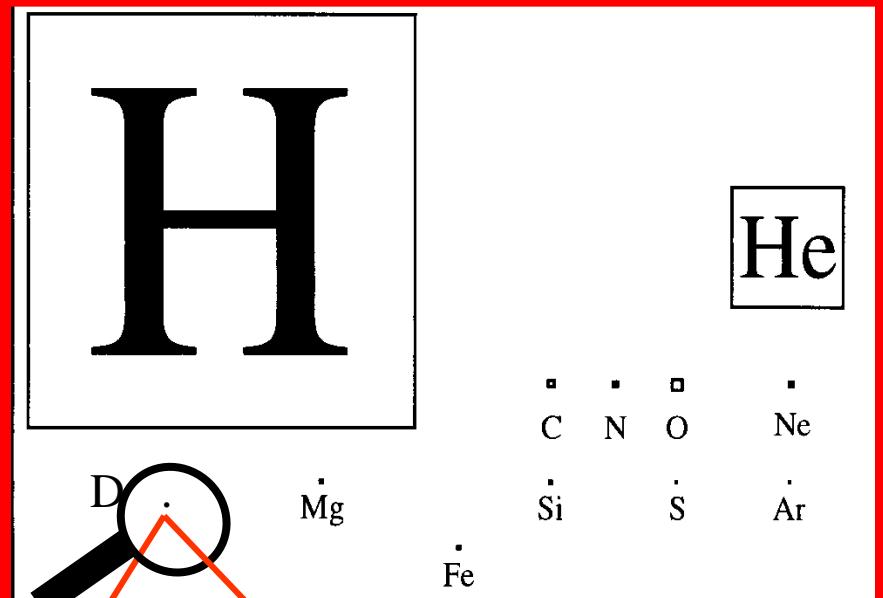
@ 10-50K

92.1% of nucleons in the universe are protons

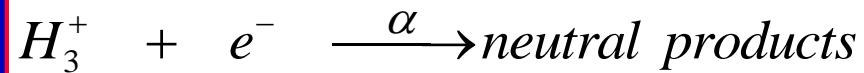
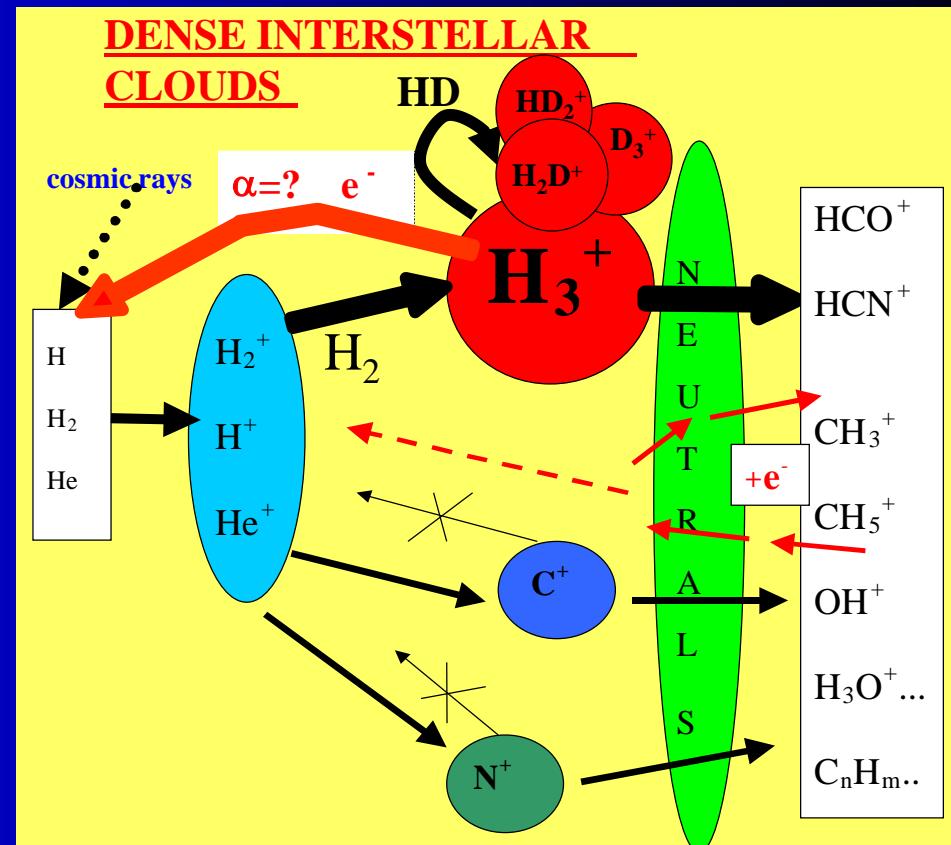
7.8% are helium nuclei !

0.1%.....C,N,O,S,Si....

Cosmic abundance



$D/H \text{ ratio} \sim 10^{-5}$

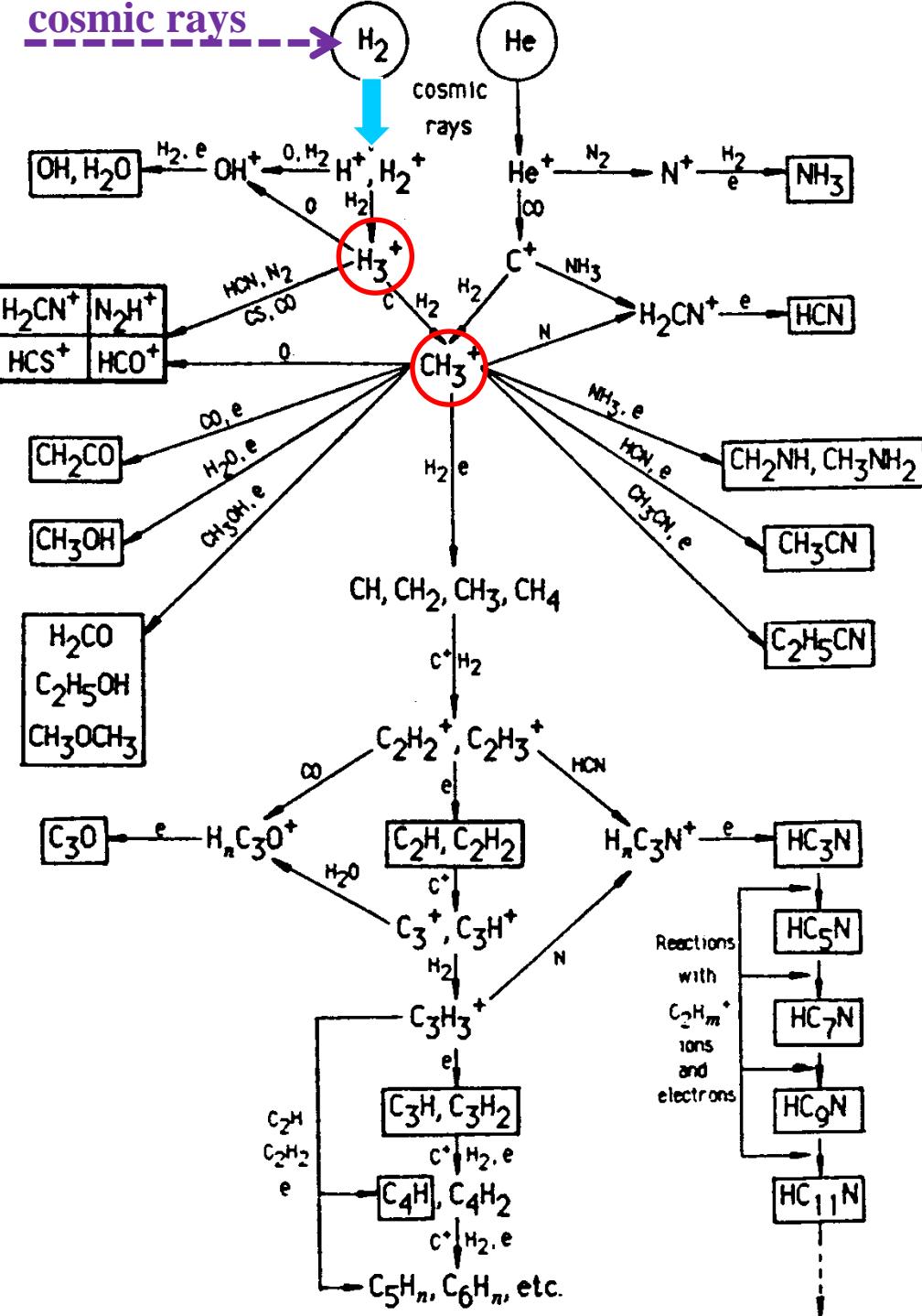
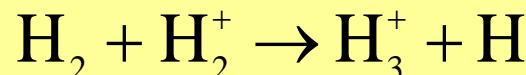
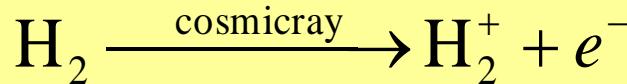


$\alpha (10 \text{ K}) = ????$

$k (10 \text{ K}) = ????$



# $\text{H}_3^+$ in interstellar space



# Observation of high population of deuterated molecules

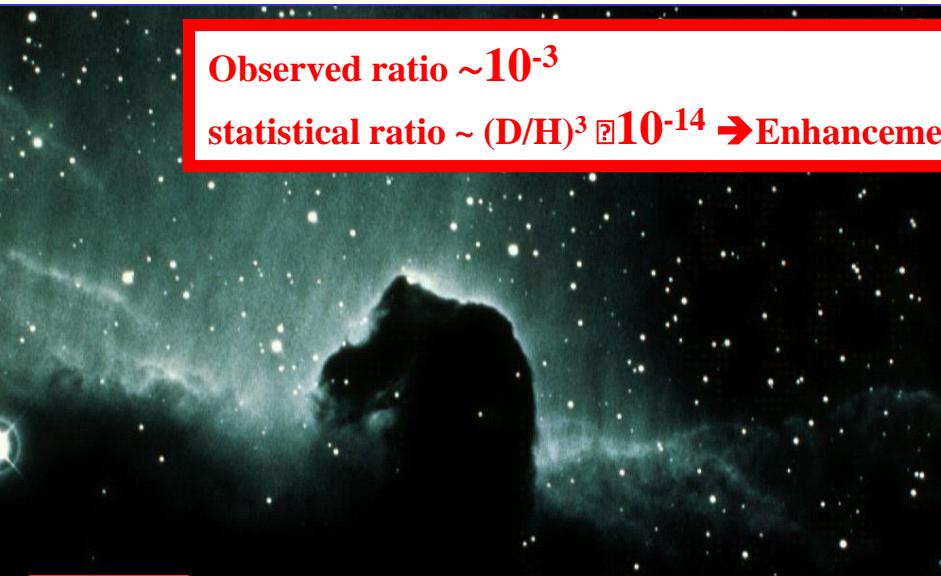
The first detection of deuterated molecules were made in the early 1970s..... Observed enhancement of D in molecules

$\text{H}_2\text{D}$	Stark	(1999)	$1_{10}-1_{11}$ transition of ortho- emission from young stellar object NGC 1333 IRAS4A.
$\text{H}_2\text{D}^+$	Caselli	(2003)	detected towards L1544.
$\text{HD}_2^+$	Vastel	(2004)	the first detection
$\text{CH}_2\text{DOH}$ ...	Parise	(2003, 2004)	have detected 4 isotopomers of deuterated methanol
$\text{NHD}_2/\text{NH}_3$	Roueff	(2000)	
	Loinard	(2001)	is 0.005 in the cold cloud L134N and 0.03 in the low-mass protostar 16293 E
$\text{D}_2\text{CO}/\text{H}_2\text{CO}$	Loinard	(2002)	
	Bacmann	(2003)	is between 0.01 and 0.4 in a low-mass protostars and prestellar cores
$\text{NH}_2\text{D}/\text{NH}_3$	J. Hatchell	(2003)	high ratios~4–33% in protostellar cores

$\text{ND}_3/\text{NH}_3$	Lis	(2002)	ratio $\sim 10^{-3}$ cold dense Barnard 1 cloud
	Tak	(2002)	Class 0 protostar NGC 1333 IRAS4A

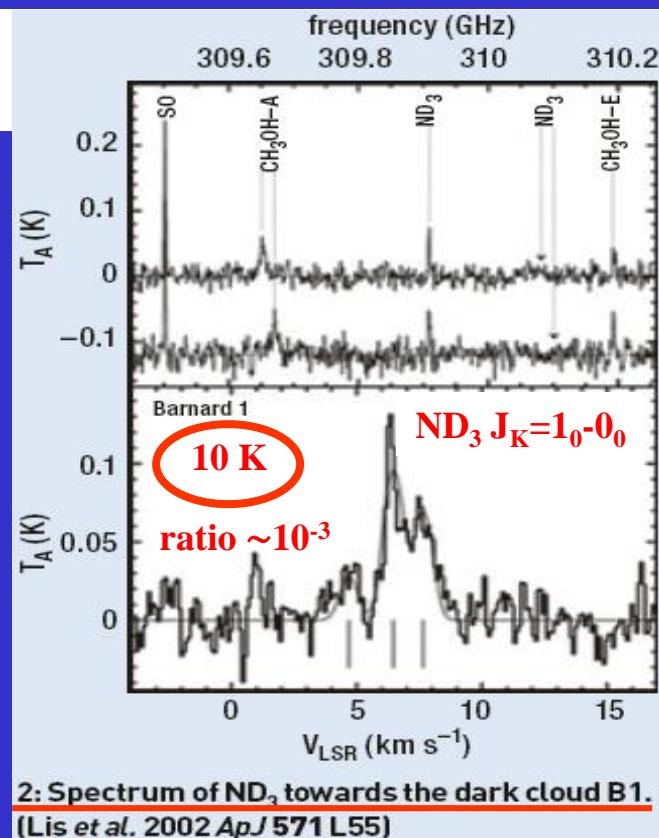
Observed ratio  $\sim 10^{-3}$

statistical ratio  $\sim (\text{D/H})^3 \approx 10^{-14} \rightarrow$  Enhancement of  $10^{11}$

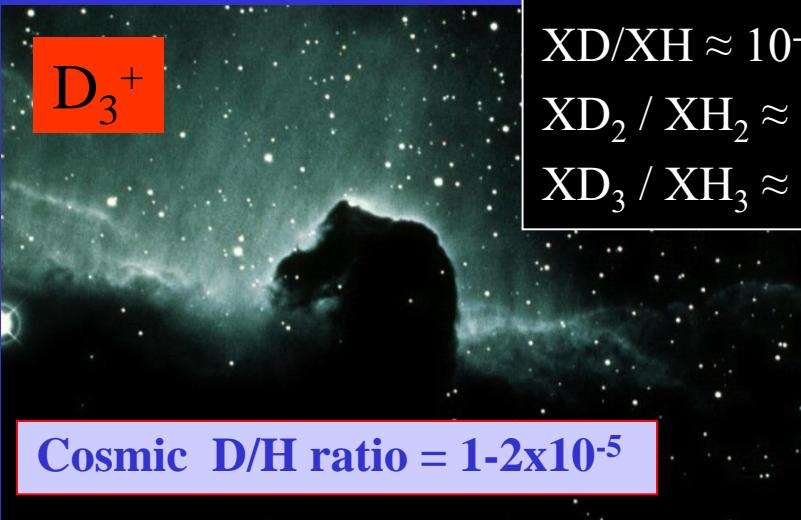


$\text{D}_3^+$

Cosmic D/H ratio =  $1-2 \times 10^{-5}$



# High population of deuterated molecules



Cosmic D/H ratio =  $1-2 \times 10^{-5}$

Cosmic D/H  $\approx 10^{-5}$   
 XD/XH  $\approx 10^{-1}-10^{-3}$   
 XD<sub>2</sub> / XH<sub>2</sub>  $\approx 10^{-2}$   
 XD<sub>3</sub> / XH<sub>3</sub>  $\approx 10^{-3}$

H <sub>3</sub> <sup>+</sup>	H <sub>2</sub> D <sup>+</sup>	D <sub>2</sub> H <sup>+</sup>	D <sub>3</sub> <sup>+</sup>
HD			
N <sub>2</sub> D <sup>+</sup>	DCO <sup>+</sup>		DCN
DNC	HDCS		D <sub>2</sub> CS
HDO	DC <sub>3</sub> N		DC <sub>5</sub> N
C <sub>3</sub> HD	HDCO		D <sub>2</sub> CO
CH <sub>3</sub> OD	CH <sub>2</sub> DOH		CHD <sub>2</sub> OH
CD <sub>3</sub> OH	CH <sub>2</sub> DCN		NH <sub>2</sub> D
NHD <sub>2</sub>	ND <sub>3</sub>		CHD <sub>2</sub> CCH
CH <sub>3</sub> CCD	C <sub>2</sub> D		C <sub>4</sub> D
HDS	D <sub>2</sub> S		

Deuterated molecules that have been detected in interstellar clouds as of February 2005.

Species	Observed ratio
NH <sub>2</sub> D/NH <sub>3</sub>	0.01
HDCO/H <sub>2</sub> CO	0.005-0.11
DCN/HCN	0.023
DNC/HNC	0.015
C <sub>2</sub> D/C <sub>2</sub> H	0.01
DCO <sup>+</sup> /HCO <sup>+</sup>	0.02
N <sub>2</sub> D <sup>+</sup> /N <sub>2</sub> H <sup>+</sup>	0.08
DC <sub>3</sub> N/HC <sub>3</sub> N	0.03-0.1
HDCS/H <sub>2</sub> CS	0.02

## Gas phase reactions,

ion-molecule reactions,  
recombination

## Grain surface reactions

Physics of condensation and evaporation from grain surface

# Deuterated gas phase molecules in space

<b>HD * #</b>	<b>HDCO</b>	<b>H<sub>2</sub>D<sup>+</sup> *</b>	<b>D<sub>2</sub>CO</b>
<b>HDO *</b>	<b>HDCS</b>	<b>DCO<sup>+</sup> *</b>	<b>ND<sub>2</sub>H</b>
<b>DCN *</b>	<b>DC<sub>3</sub>N</b>	<b>N<sub>2</sub>D<sup>+</sup></b>	<b>CHD<sub>2</sub>OH</b>
<b>DNC</b>	<b>CH<sub>2</sub>DOH</b>		<b>D<sub>2</sub>S</b>
<b>HDS</b>	<b>CH<sub>3</sub>OD</b>		<b>ND<sub>3</sub></b>
<b>C<sub>2</sub>D</b>	<b>DC<sub>5</sub>N</b>		<b>CD<sub>3</sub>OH</b>
<b>C<sub>4</sub>D</b>	<b>CH<sub>2</sub>DCCCH</b>		<b>D<sub>2</sub>CS</b>
<b>C<sub>3</sub>HD</b>	<b>CH<sub>2</sub>DCN</b>		
<b>NH<sub>2</sub>D</b>	<b>CH<sub>3</sub>D</b>		

**Planets**

**Comets**

**CS disks**

**ISM**

**Extragalactic #**

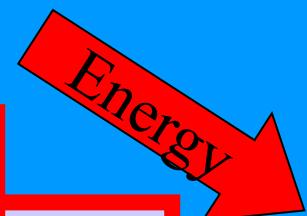
Cosmic D/H  $\approx 10^{-5}$

XD/XH  $\approx 10^{-1}$ - $10^{-3}$

XD<sub>2</sub> / XH<sub>2</sub>  $\approx 10^{-2}$

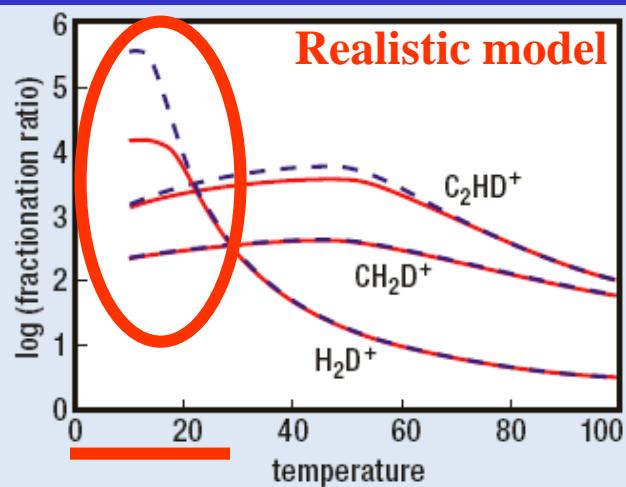
XD<sub>3</sub> / XH<sub>3</sub>  $\approx 10^{-3}$

**HD**

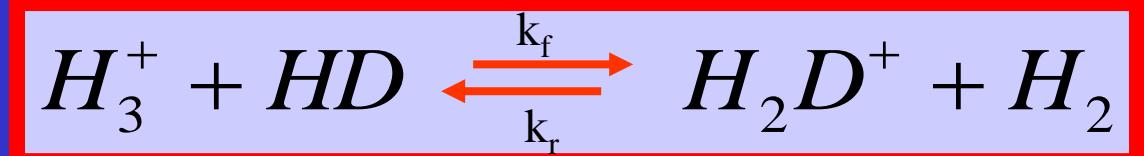


# Small differences in zero point energies for deuterated molecules

$$\Delta H / k = -232 \text{ K}$$



3: The enhancement in the fractionation of primary ions relative to the HD/H<sub>2</sub> ratio as a function of temperature in interstellar clouds

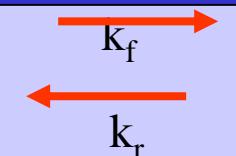


$$\frac{k_r}{k_f} \sim \exp(\Delta H / kT) \sim \exp(-232 / T)$$

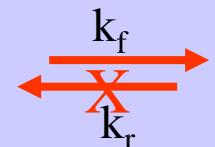
In equilibrium

$$\frac{\text{H}_3^+}{\text{H}_2\text{D}^+} = \frac{\text{H}_2}{\text{HD}} \frac{k_r}{k_f}$$

$$@ 300 \text{ K} \quad \frac{k_r}{k_f} \sim \exp(-1) \sim 0.4$$



$$@ 10 \text{ K} \quad \frac{k_r}{k_f} \sim \exp(-23) \sim 10^{-10}$$



$$@ 10 \text{ K} \quad \frac{\text{H}_3^+}{\text{H}_2\text{D}^+} = \frac{\text{H}_2}{\text{HD}} \frac{k_r}{k_f} \sim 10^5 \cdot 10^{-10} = 10^{-5}$$

ONLY PARTLY !!!???

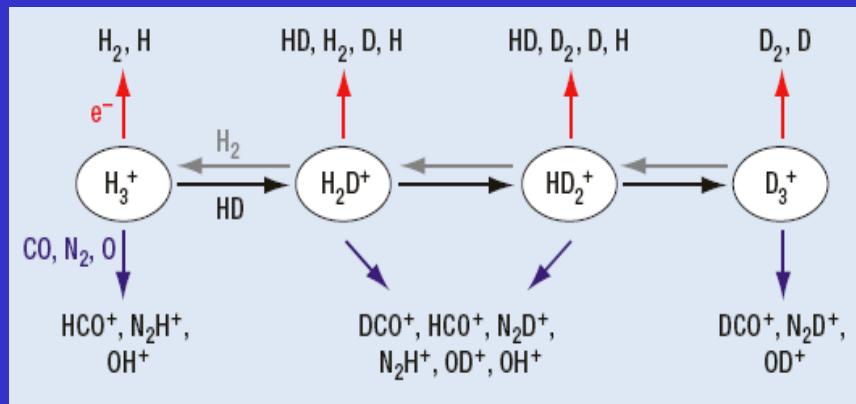


$$-\Delta H / k$$

$$187 \text{ K}$$



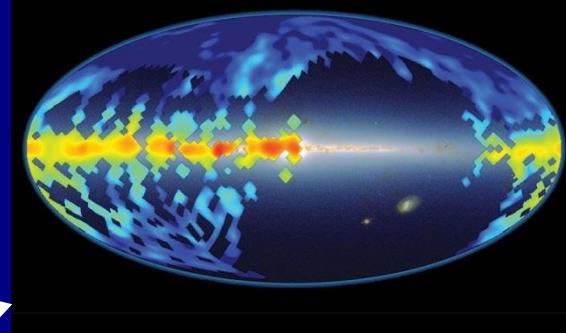
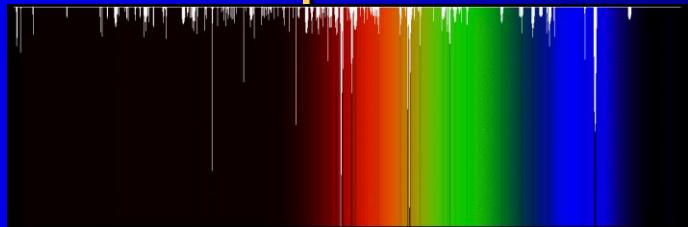
$$234 \text{ K}$$



# Molecules in interstellar space

DIBs - diffuse bands

1919-1922



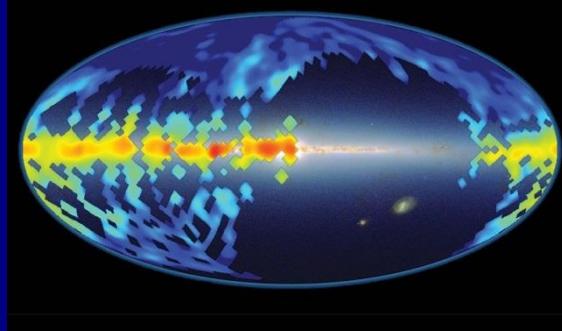
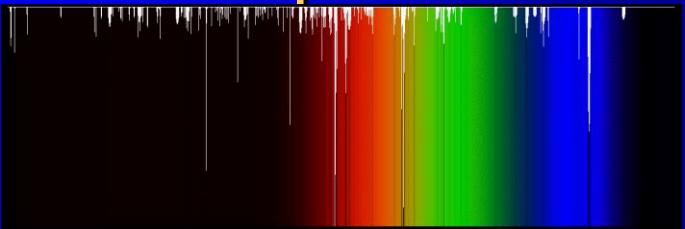
## 1919-1922 Heger discovers the DIBs

Nearly 100 years ago Mary Lea Heger discovered diffuse bands in the spectra of stars due to some sort of material maybe molecules in the space between stars and Earth. A map of the data from the Sloan Digital Sky Survey, by a team from Johns Hopkins produced this map. **Red indicates areas with the most abundant DIB molecules, blue the least.**

# Molecules in interstellar space

DIBs - diffuse bands

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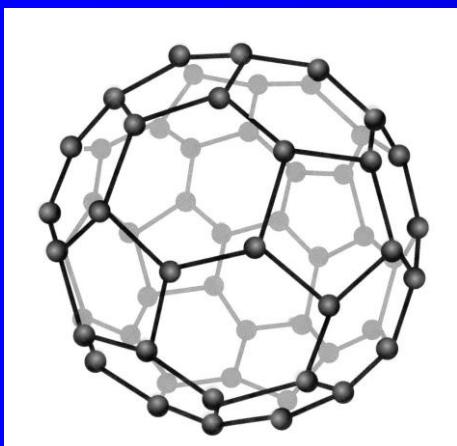
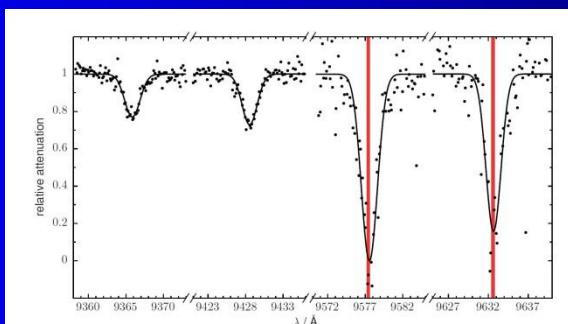
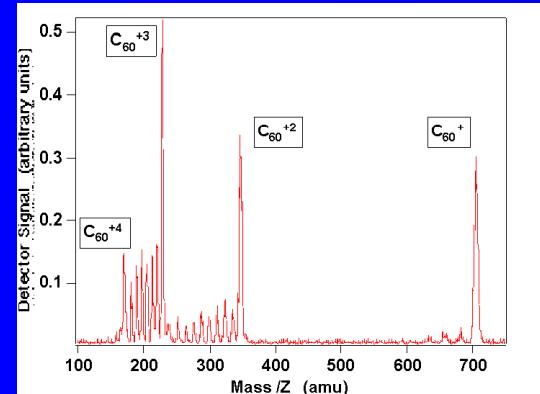
16 JULY 2015 | VOL 523 | NATURE | 323

LETTER 2015

doi:10.1038/nature14566

## Laboratory confirmation of $C_{60}^+$ as the carrier of two diffuse interstellar bands

E. K. Campbell<sup>1</sup>, M. Holz<sup>1</sup>, D. Gerlich<sup>2</sup> & J. P. Maier<sup>1</sup>

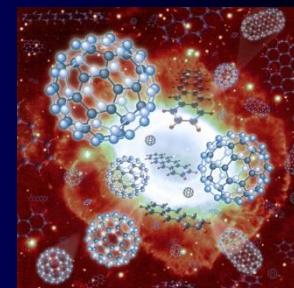
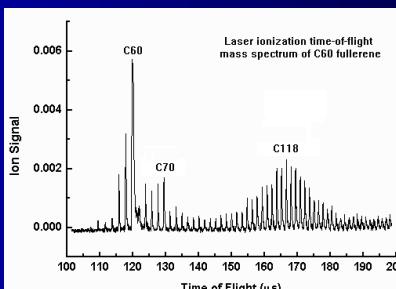


RESEARCH NEWS & VIEWS

ASTROCHEMISTRY

## Fullerene solves an interstellar puzzle

Laboratory measurements confirm that a 'buckyball' ion is responsible for two near-infrared absorption features found in spectra of the interstellar medium, casting light on a century-old astrochemical mystery. SEE LETTER P.323



# Observation of H<sub>2</sub>O<sup>+</sup>

A&A 550, A25 (2013)  
DOI: 10.1051/0004-6361/201220466  
© ESO 2013

2013

Astronomy  
&  
Astrophysics

## Excited OH<sup>+</sup>, H<sub>2</sub>O<sup>+</sup>, and H<sub>3</sub>O<sup>+</sup> in NGC 4418 and Arp 220\*

E. González-Alfonso<sup>1</sup>, J. Fischer<sup>2</sup>, S. Bruderer<sup>3</sup>, H. S. P. Müller<sup>4</sup>, J. Graciá-Carpio<sup>3</sup>, E. Sturm<sup>3</sup>, D. Lutz<sup>3</sup>, A. Poglitsch<sup>3</sup>, H. Feuchtgruber<sup>3</sup>, S. Veilleux<sup>5,6</sup>, A. Contursi<sup>7</sup>, A. Sternberg<sup>7</sup>, S. Hailey-Dunsheath<sup>8</sup>, A. Verma<sup>9</sup>, N. Christopher<sup>9</sup>, R. Davies<sup>3</sup>, R. Genzel<sup>3</sup>, and L. Tacconi<sup>3</sup>

\* *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.



**Herschel**

7,5 metru dlouhý a 4 m široký.  
Vážil 3400 kg

Start	14. května 2009 v 13:12:02 UTC
Kosmodrom	kosmodrom v Kourou, Francouzská Guyana <sup>[1]</sup>
Nosná raketa	Ariane 5 <sup>[1]</sup>
Stav objektu	obíhala Librační bod L <sub>2</sub> <sup>[1]</sup>
Trvání mise	17. června 2013 3 až 4 roky <sup>[1]</sup>

## ABSTRACT

We report on *Herschel*/PACS observations of absorption lines of OH<sup>+</sup>, H<sub>2</sub>O<sup>+</sup> and H<sub>3</sub>O<sup>+</sup> in NGC 4418 and Arp 220. Excited lines of OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> with  $E_{\text{lower}}$  of at least 285 and  $\sim 200$  K, respectively, are detected in both sources, indicating radiative pumping and location in the high radiation density environment of the nuclear regions. Abundance ratios OH<sup>+</sup>/H<sub>2</sub>O<sup>+</sup> of 1–2.5 are estimated in the nuclei of both sources. The inferred OH<sup>+</sup> column and abundance relative to H nuclei are  $(0.5\text{--}1) \times 10^{16}$  cm<sup>-2</sup> and  $\sim 2 \times 10^{-8}$ , respectively. Additionally, in Arp 220, an extended low excitation component around the nuclear region is found to have OH<sup>+</sup>/H<sub>2</sub>O<sup>+</sup>  $\sim 5\text{--}10$ . H<sub>3</sub>O<sup>+</sup> is detected in both sources with  $N(\text{H}_3\text{O}^+) \sim (0.5\text{--}2) \times 10^{16}$  cm<sup>-2</sup>, and in Arp 220 the pure inversion, metastable lines indicate a high rotational temperature of  $\sim 500$  K, indicative of formation pumping and/or hot gas. Simple chemical models favor an ionization sequence dominated by  $\text{H}^+ \rightarrow \text{O}^+ \rightarrow \text{OH}^+ \rightarrow \text{H}_2\text{O}^+ \rightarrow \text{H}_3\text{O}^+$ , and we also argue that the H<sup>+</sup> production is most likely dominated by X-ray/cosmic ray ionization. The full set of observations and models leads us to propose that the molecular ions arise in a relatively low density ( $\gtrsim 10^4$  cm<sup>-3</sup>) interclump medium, in which case the ionization rate per H nucleus (including secondary ionizations) is  $\zeta > 10^{-13}$  s<sup>-1</sup>, a lower limit that is several  $\times 10^2$  times the highest current rate estimates for Galactic regions. In Arp 220, our lower limit for  $\zeta$  is compatible with estimates for the cosmic ray energy density inferred previously from the supernova rate and synchrotron radio emission, and also with the expected ionization rate produced by X-rays. In NGC 4418, we argue that X-ray ionization due to an active galactic nucleus is responsible for the molecular ion production.

## Modeling observations of the interstellar medium (ISM)

David Neufeld  
Johns Hopkins University

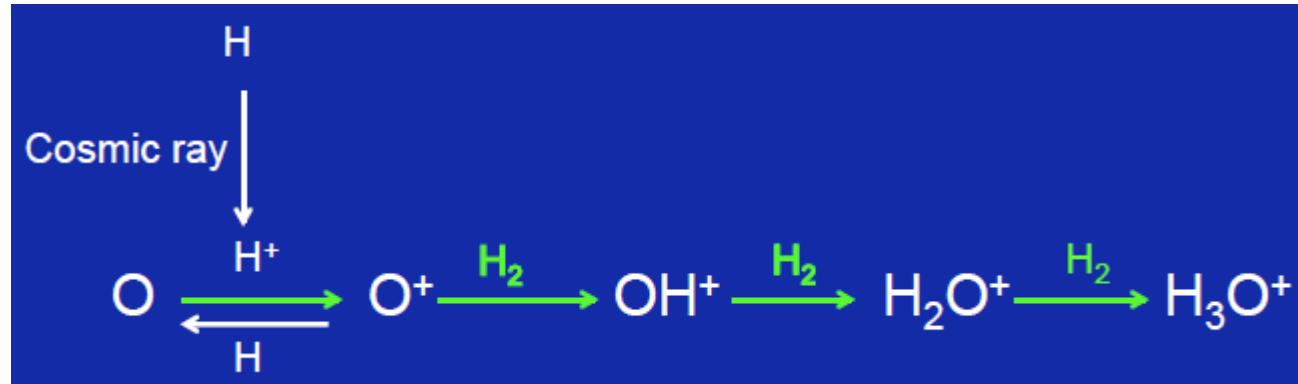
### Measuring the cosmic-ray ionization rate with OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup>

Unlike C<sup>+</sup> and S<sup>+</sup>, O<sup>+</sup> does react with H<sub>2</sub> at low temperature. But O is not ionized by UV radiation longward of the Lyman limit, so OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> formation must be initiated by cosmic ray ionization

## Recent discoveries of molecules in the diffuse ISM

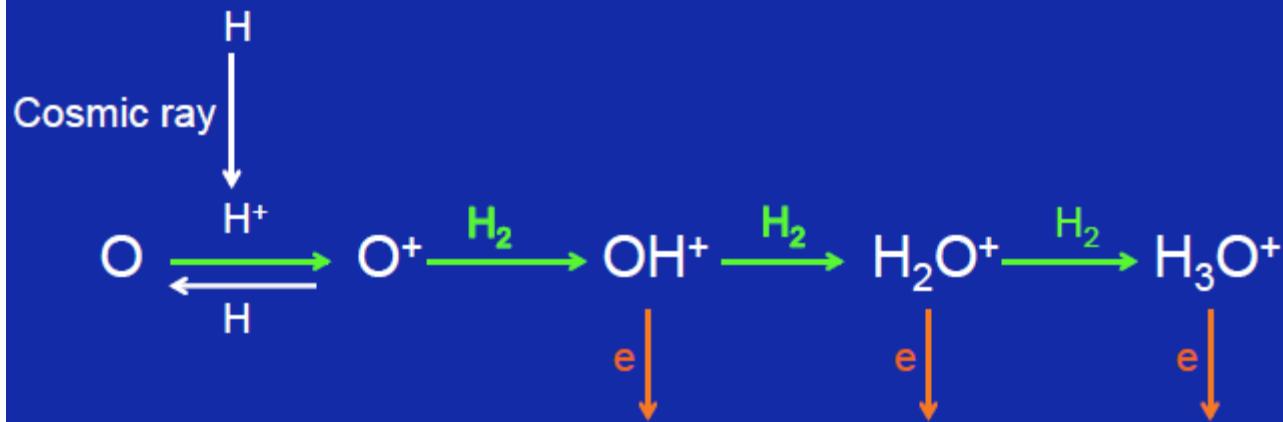
OH <sup>+</sup>	Wyrowski et al. 2010	APEX
SH <sup>+</sup>	Menten et al. 2011	APEX
H <sub>2</sub> O <sup>+</sup>	Gerin et al. 2010	Herschel
HF	Neufeld et al. 2010	Herschel
HCl <sup>+</sup>	de Luca et al. 2013	Herschel
H <sub>2</sub> Cl <sup>+</sup>	Lis et al. 2010	Herschel
SH	Neufeld et al. 2012	SOFIA
ArH <sup>+</sup>	Schilke et al. 2014	Herschel

All hydrides with high frequency rotational transitions that are unobservable from the ground or observable only from superb submillimeter sites



# Determining the molecular fraction in the diffuse ISM

The OH<sup>+</sup>/H<sub>2</sub>O<sup>+</sup> ratio reflects a competition between reaction of OH<sup>+</sup> with H<sub>2</sub> and reaction with electrons



Observed OH<sup>+</sup>/H<sub>2</sub>O<sup>+</sup> ratios ~ 3 to 15 imply that only 2 – 10 % of the H is typically in H<sub>2</sub>



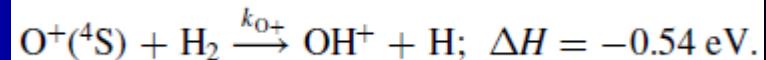
2018

## OH<sup>+</sup> Formation in the Low-temperature O<sup>+(4S)</sup> + H<sub>2</sub> Reaction

Artem Kovalenko , Thuy Dung Tran , Serhiy Rednyk , Štěpán Roučka , Petr Dohnal , Radek Plašil , Dieter Gerlich , and Juraj Glosík

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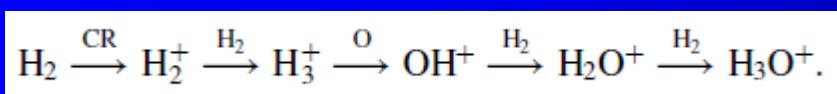
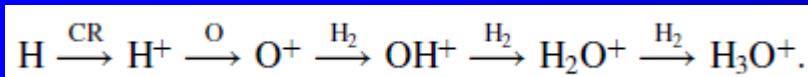
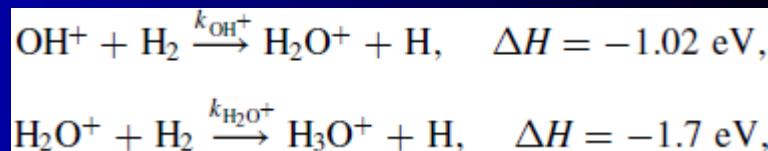
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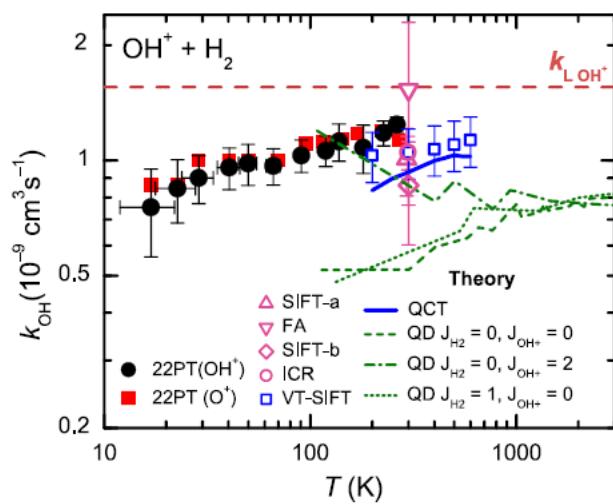
## Formation of H<sub>2</sub>O<sup>+</sup> and H<sub>3</sub>O<sup>+</sup> Cations in Reactions of OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> with H<sub>2</sub>: Experimental Studies of the Reaction Rate Coefficients from T = 15 to 300 K

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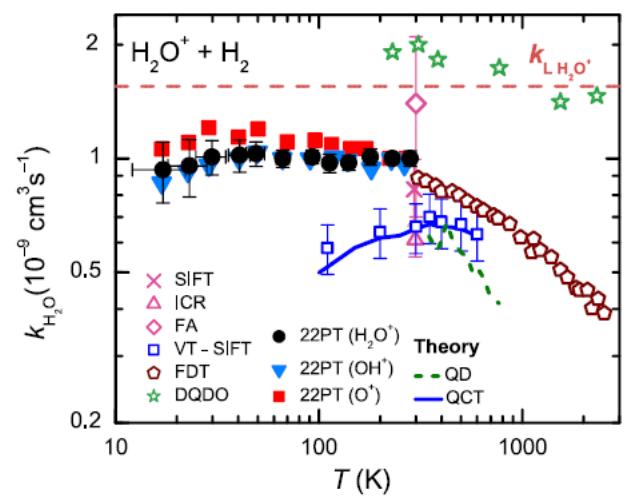
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**Figure 4.** Temperature dependence of the rate coefficient  $k_{\text{OH}^+}$  of the reaction of  $\text{OH}^+$  with normal hydrogen. The averaged data obtained in experiments with  $\text{OH}^+$  and  $\text{O}^+$  ions injected into the trap are indicated by full circles and squares, respectively. The systematic error due to pressure measurement is 20%. The dashed horizontal line ( $k_{\text{L}, \text{OH}^+}$ ) indicates the Langevin collisional rate coefficient. The previous results at 300 K are FA (Fehsenfeld et al. 1967), ICR (Kim et al. 1975), SIFT-a (Jones et al. 1981), and SIFT-b (Shul et al. 1988). The temperature dependencies of  $k_{\text{OH}^+}$  calculated (QCT) and measured (VT-SIFT) by Martinez et al. (2015) are indicated by the full line and open squares, respectively. The dashed, dotted, and dash-dotted lines represent the phenomenological rate coefficients ( $v\sigma$ ) derived from the theoretical QD cross-sections (Song et al. 2016a) corresponding to different rotational states of reactants as indicated in the legend.



**Figure 5.** Temperature dependence of the reaction rate coefficient  $k_{\text{H}_2\text{O}^+}$  of the reaction of  $\text{H}_2\text{O}^+$  with normal hydrogen. The averaged data obtained in experiments with  $\text{H}_2\text{O}^+$ ,  $\text{OH}^+$ , and  $\text{O}^+$  ions injected into the trap are indicated by full circles, triangles, and squares, respectively. The systematic error due to pressure determination is 20%. The dashed horizontal line ( $k_{\text{L}, \text{H}_2\text{O}^+}$ ) indicates the Langevin collisional rate coefficient. The previous results at 300 K are FA (Fehsenfeld et al. 1967), ICR (Kim et al. 1975), FDT (Dotan et al. 1980), and SIFT (Jones et al. 1981). The values measured (VT-SIFT) and calculated (QCT) by Ard et al. (2014) are indicated by the open squares and by the full line (QCT), respectively. The dashed line and stars represent the phenomenological rate coefficients ( $v\sigma$ ) derived from the theoretical QD, and experimental DQDO cross-sections (Song et al. 2016b). The uncertainty of the DQDO results is 50%.

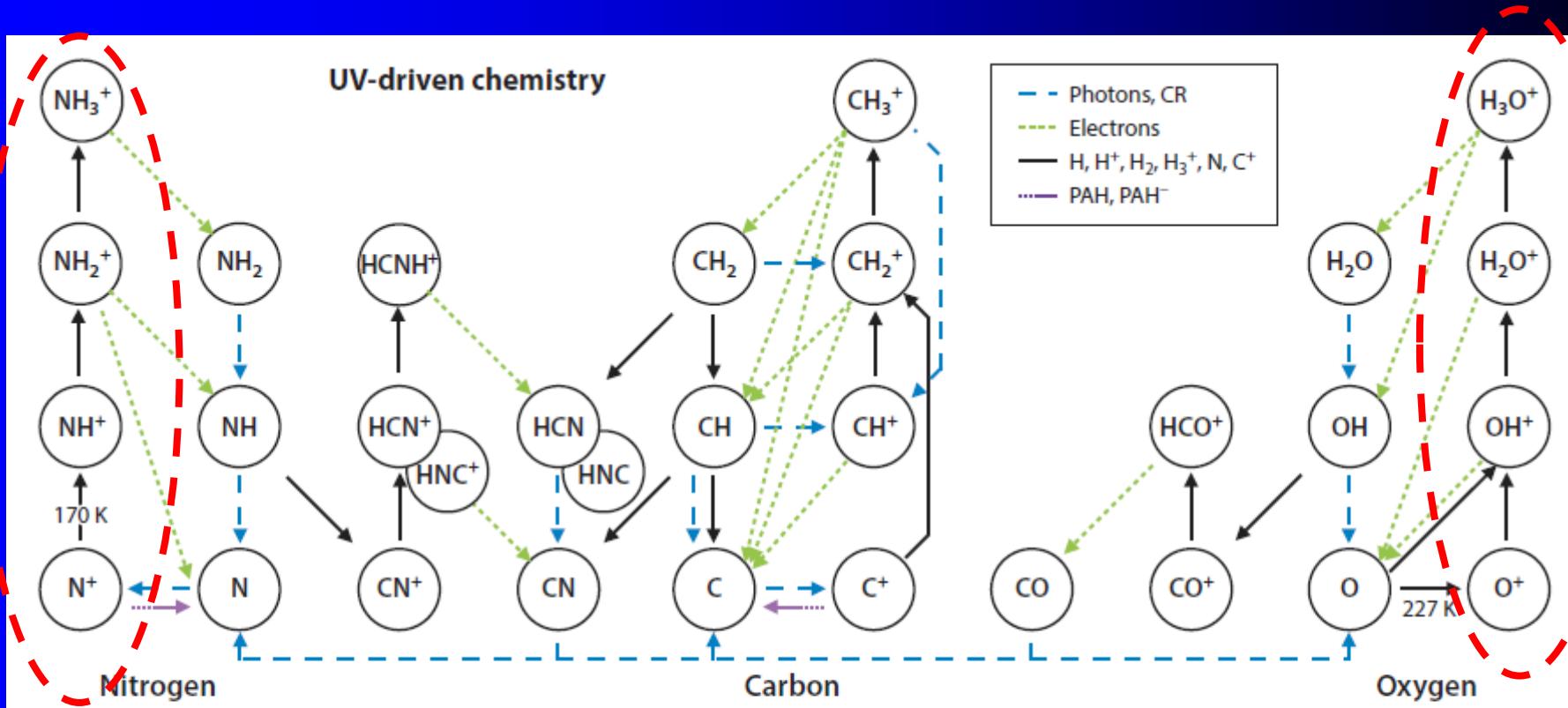
# Interstellar Hydrides

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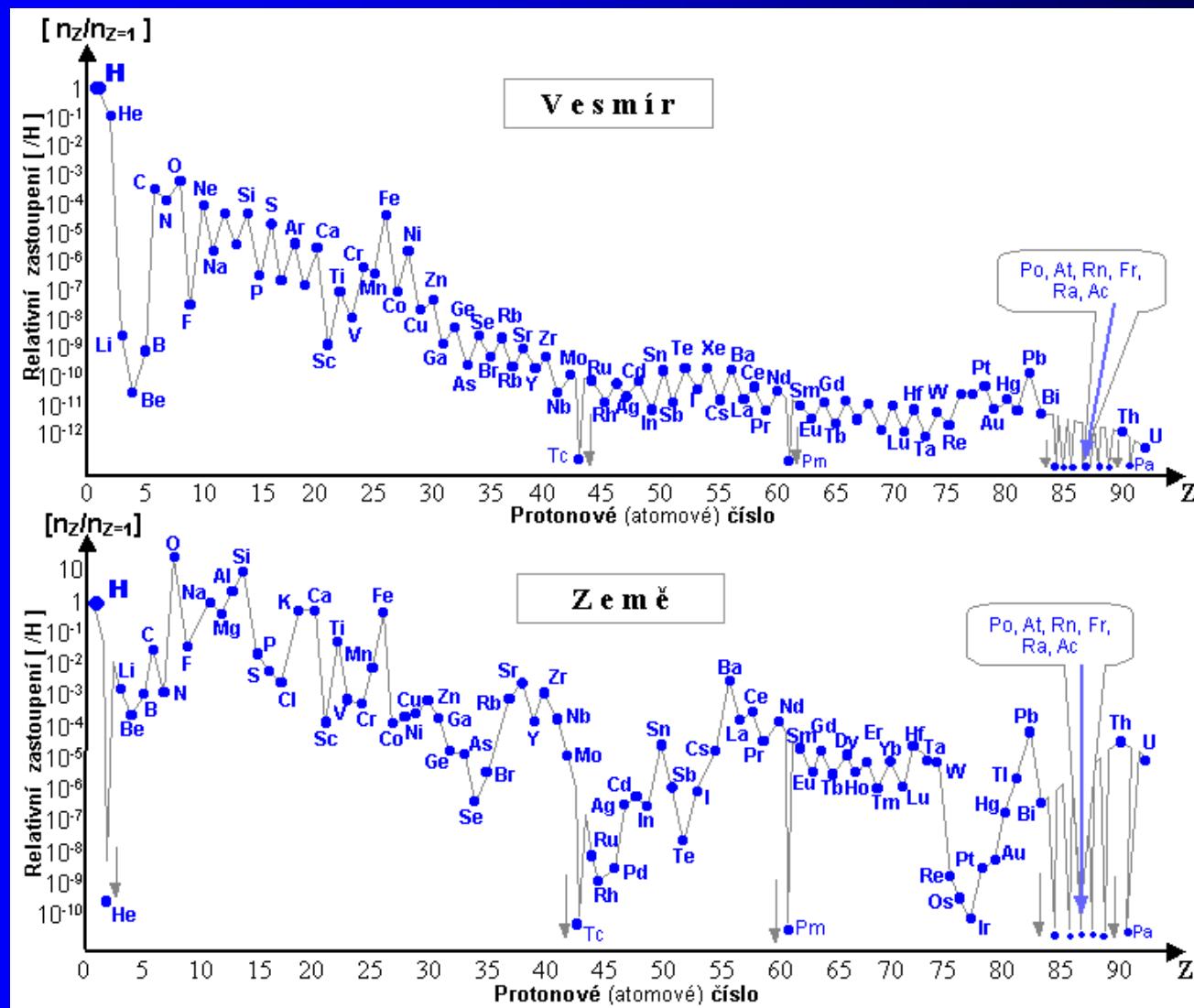
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**Figure 3**

Illustration of the chemical network initiating the carbon, oxygen, and nitrogen chemistry in diffuse cloud conditions ( $n_{\text{H}} = 50 \text{ cm}^{-3}$ ,  $A_V = 0.4 \text{ mag}$ ,  $\chi = 1$ ). The black arrows show the reactions with  $\text{H}$ ,  $\text{H}^+$ ,  $\text{H}_2$ ,  $\text{H}_3^+$ ,  $\text{C}^+$ , and  $\text{N}$ , with values of the endothermicity for the reaction between  $\text{N}^+$  and  $\text{H}_2$  and for the charge exchange reaction between  $\text{O}$  and  $\text{H}^+$ . Note that  $\text{CH}_2^+$  is formed in the slow radiative association reaction between  $\text{C}^+$  and  $\text{H}_2$ . The dashed blue arrows indicate the reactions induced by FUV photons or cosmic rays (CR). Dissociative recombination reactions with electrons are shown with green dotted arrows. Purple arrows show the neutralization reactions on dust grains and polycyclic aromatic hydrocarbons (PAHs). Adapted from Godard et al. (2014) with permission.



Relativní zastoupení prvků v přírodě v závislosti na jejich protonovém (atomovém) čísle  $Z$ , vztažené k vodíku  $Z=1$ .

**Nahoře:** Nynější průměrné zastoupení prvků ve vesmíru. **Dole:** Výskyt prvků na Zemi (v zemské kůře) a terestrických planetách.

Vzhledem k velkému rozpětí hodnot je relativní zastoupení prvků (vztažené k vodíku  $Z=1$ ) na svislé ose vyneseno v logaritmickém měřítku; to ale může zvláště na horním grafu opticky zkreslit velký rozdíl v zastoupení vodíku a helia oproti těžším prvkům..