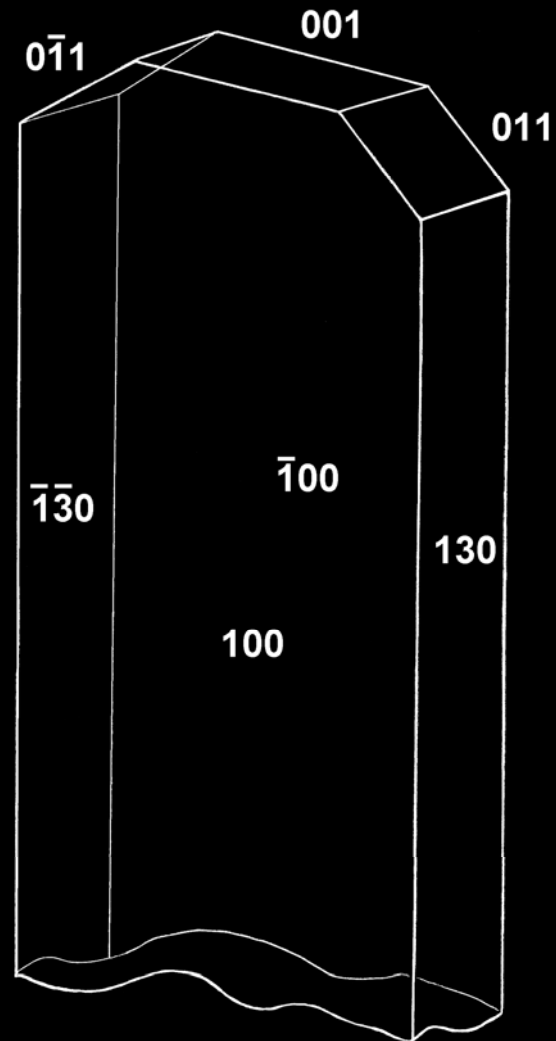
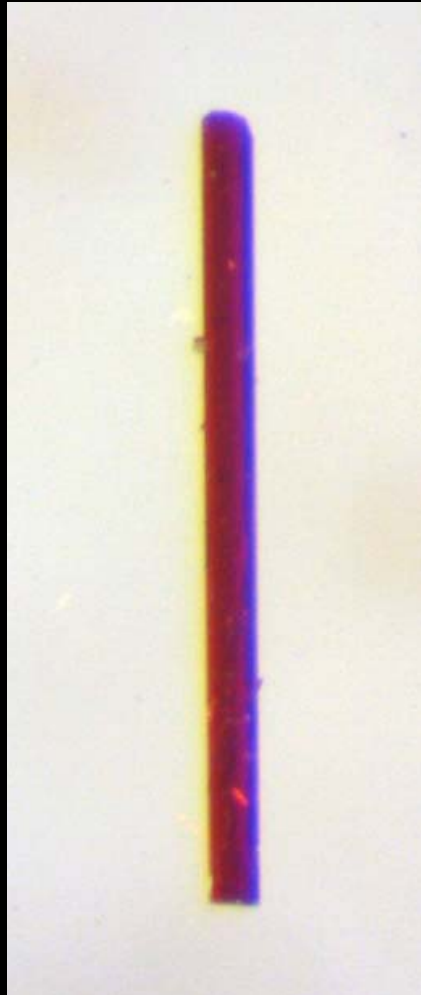


Prvih sto godina rendgenske strukturne analize

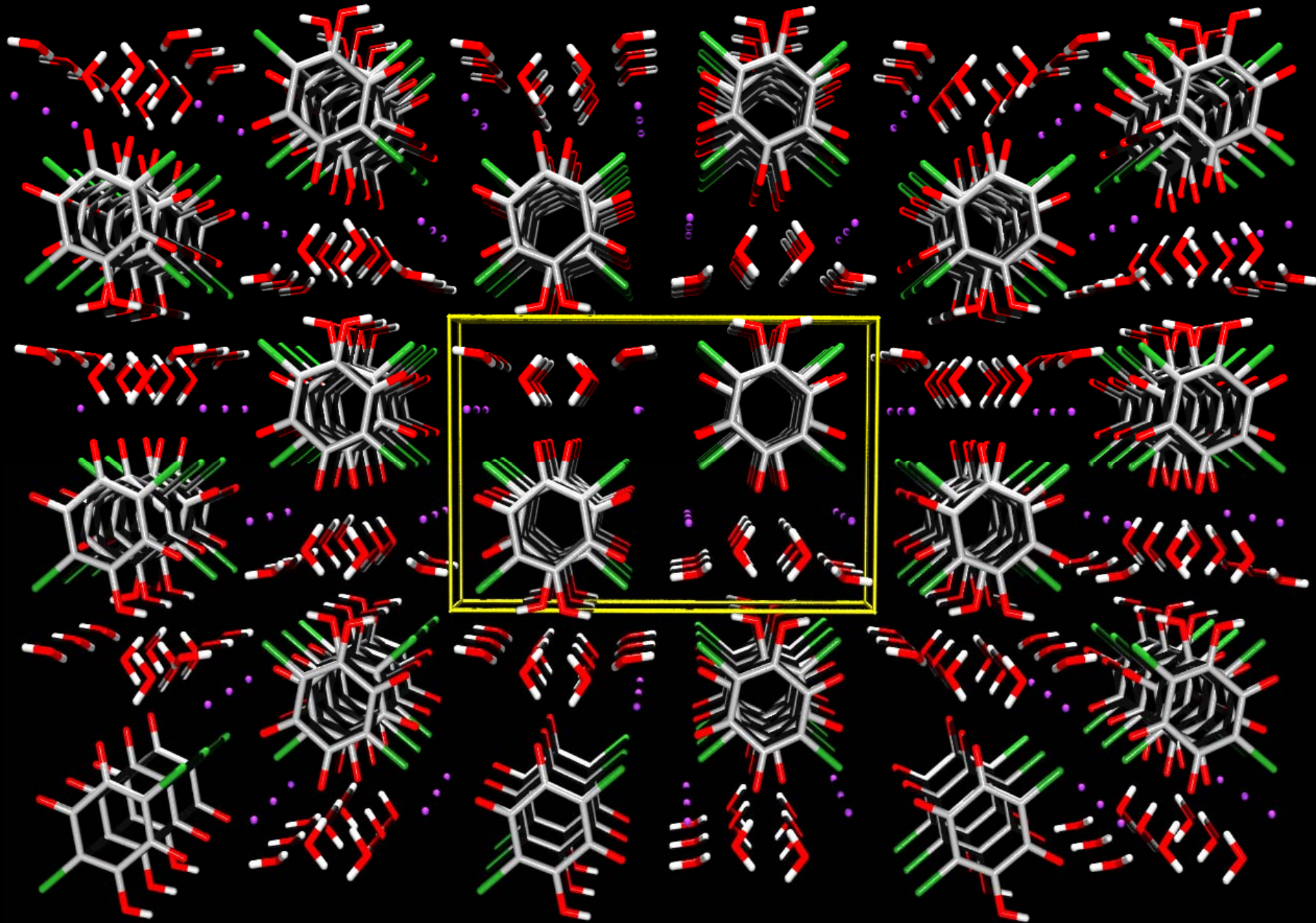
Krešimir Molčanov
Insitut “Ruđer Bošković”



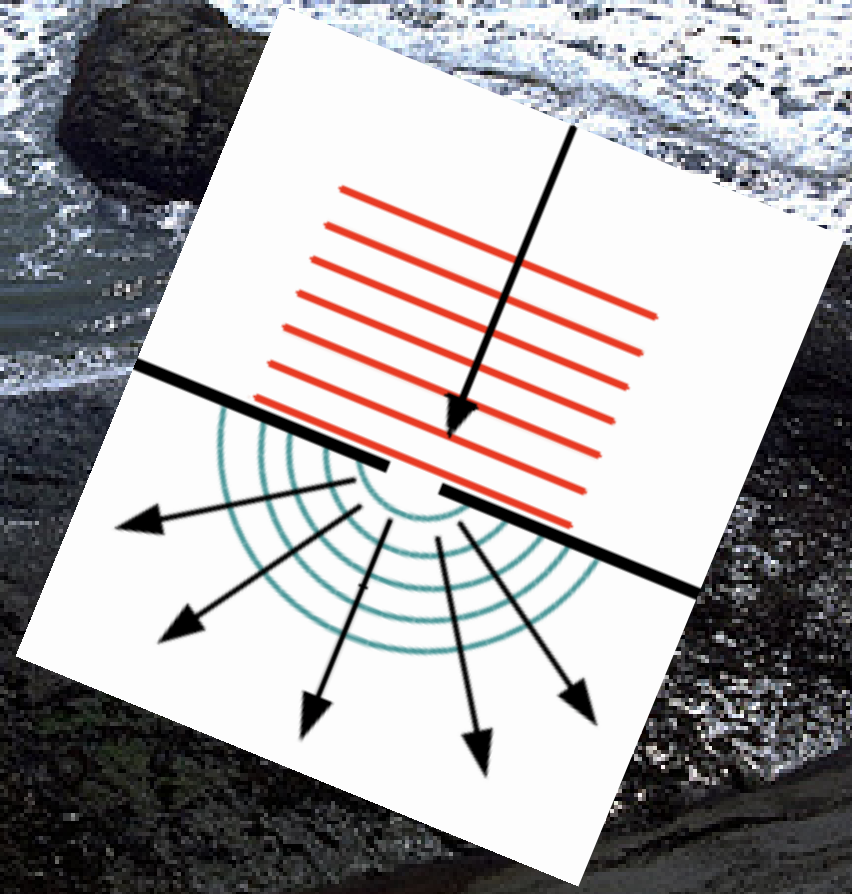
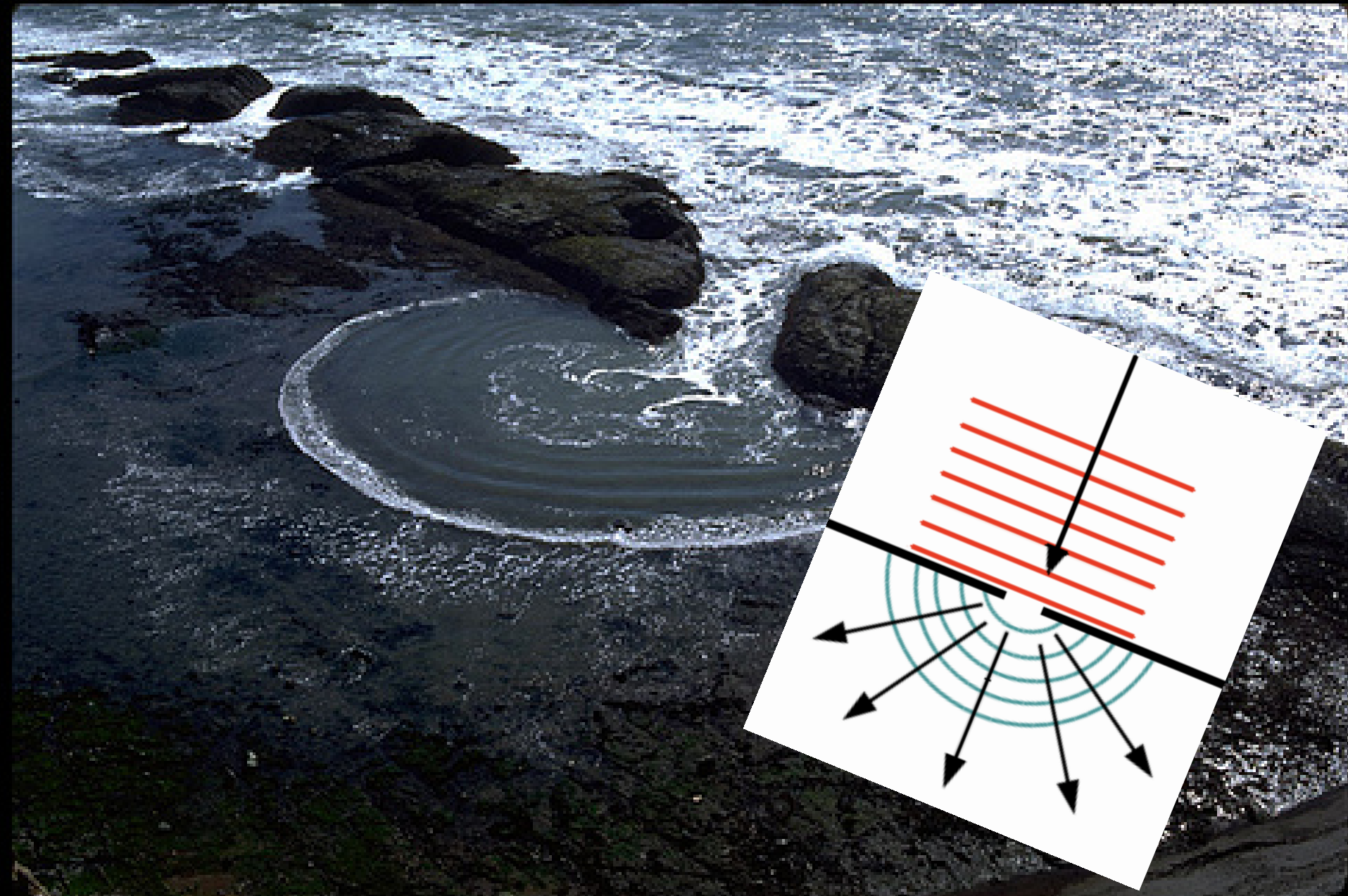
Klasična kristalografija (prije rendgena)



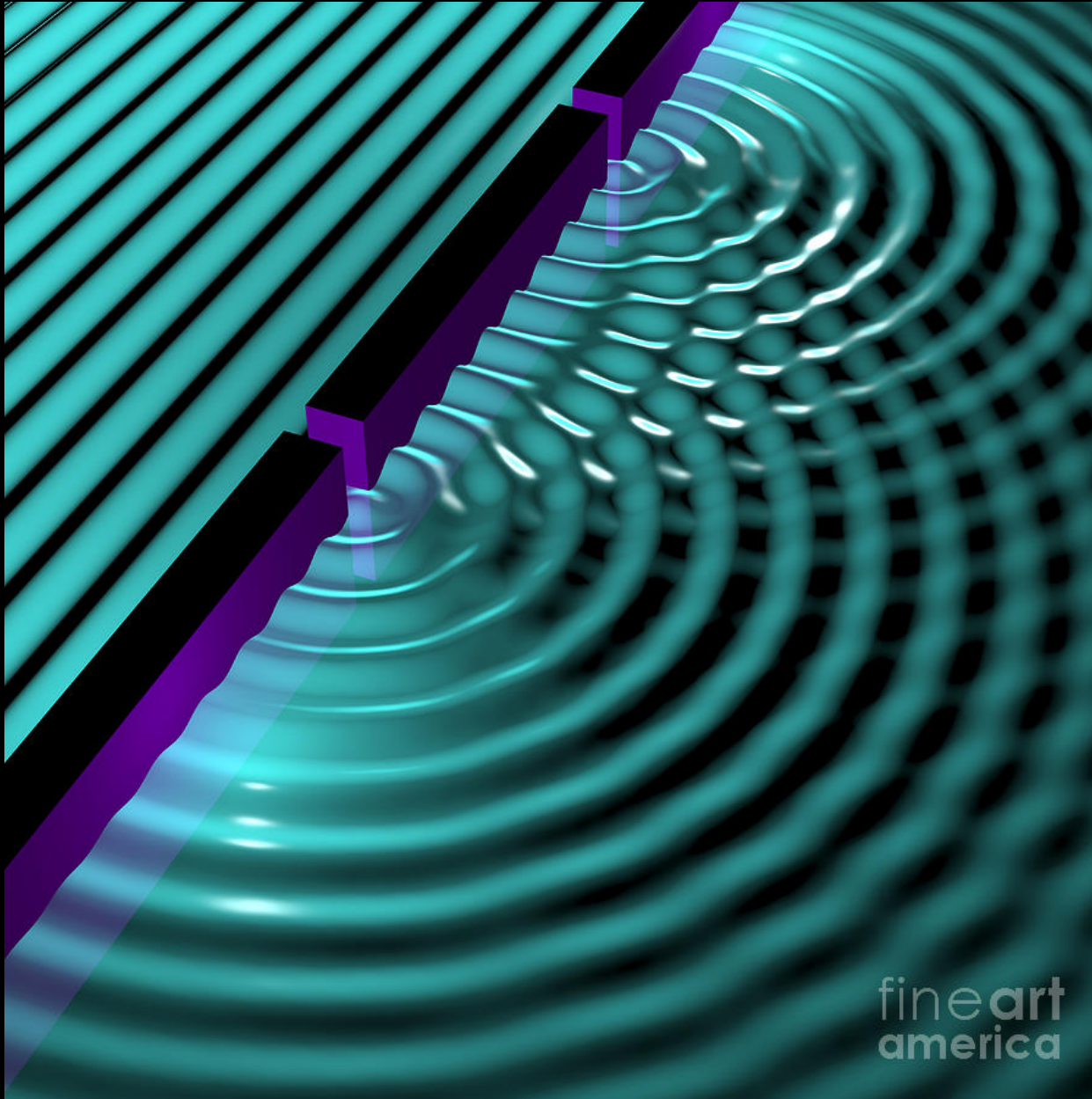
Kristal “iznutra”



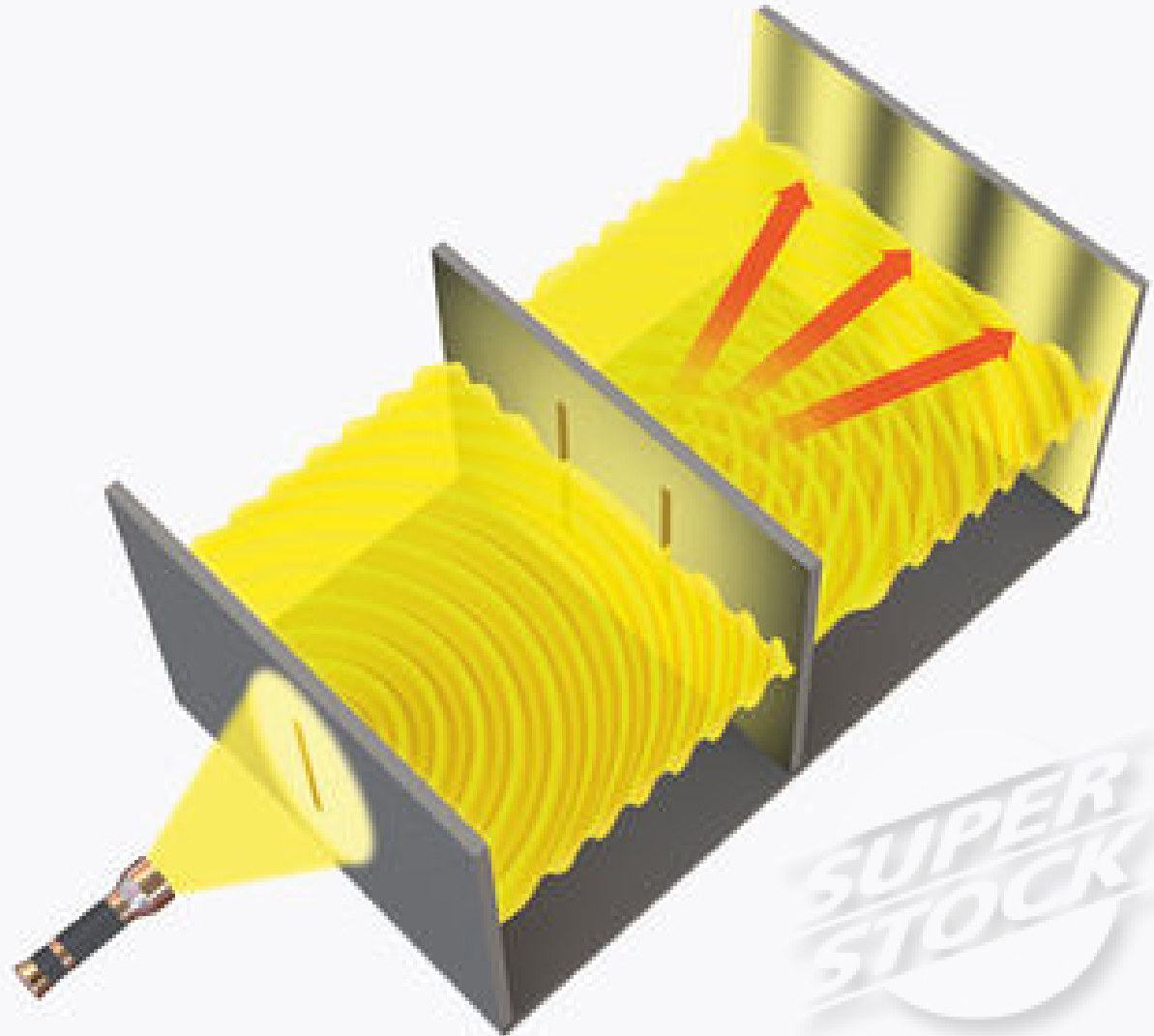
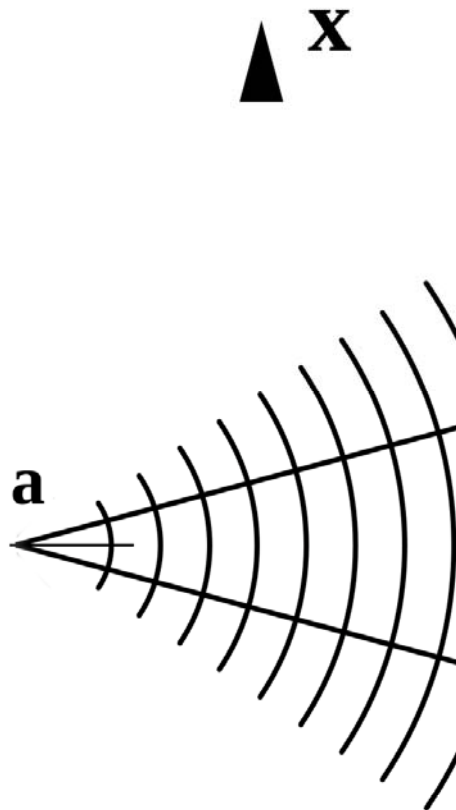
Ogib valova



Difrakcija: ogib i interferencija

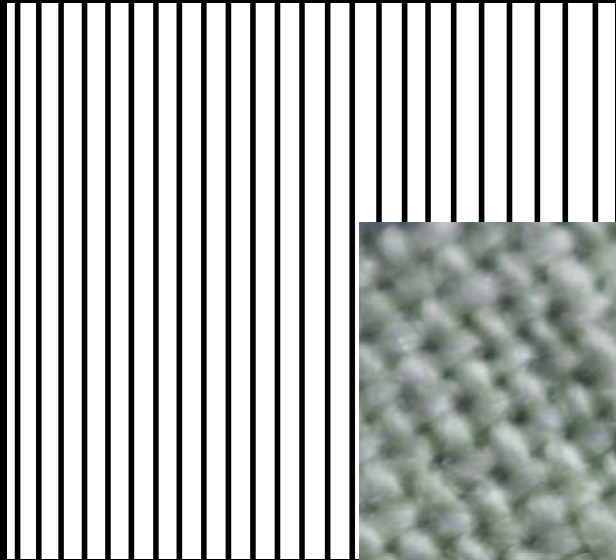


Youngov pokus (1803.)



**SUPER
STOCK**
superstock.com

Optická rešetka

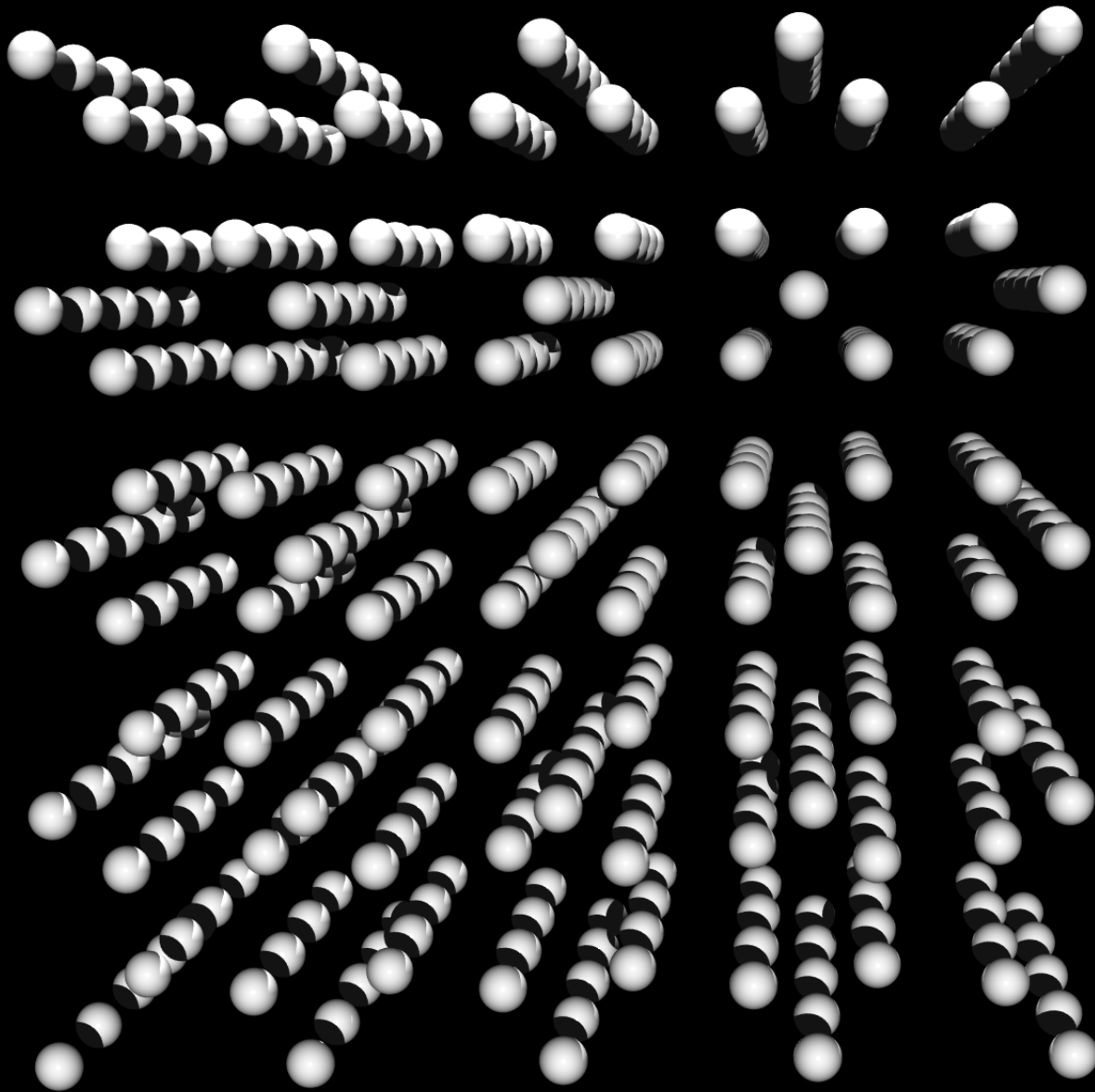


1D

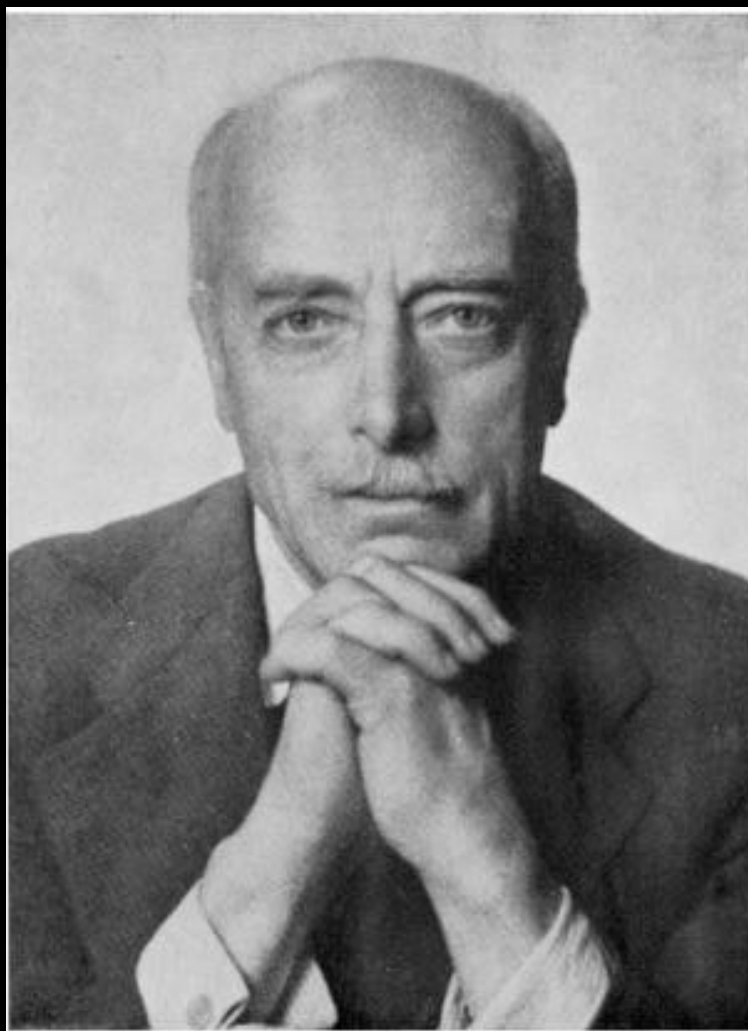
2D



Kristal: 3D optička rešetka



Prvi difrakcijski pokus



Teorija:

Max von Laue (1879.-1960.)

Eksperiment:

**W. Friedrich i P. Knipping
oko Uskrsa 1912.,
kristal modre galice**

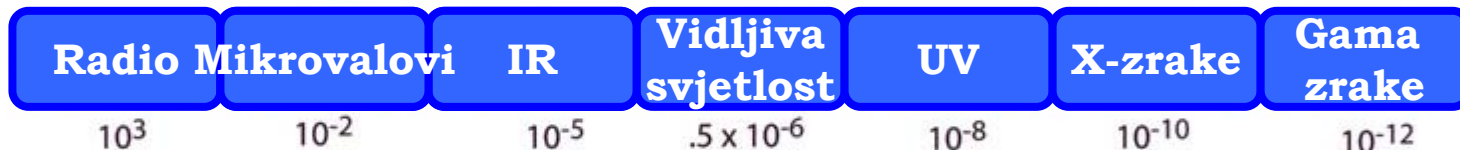
Nobelova nagrada 1914.

Elektromagnetsko zračenje

Prolazi kroz atmosferu



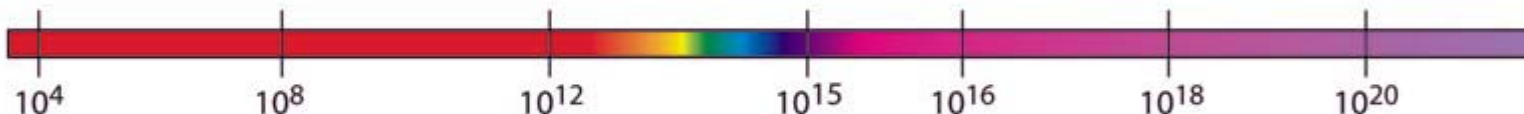
Valna duljina (metri)



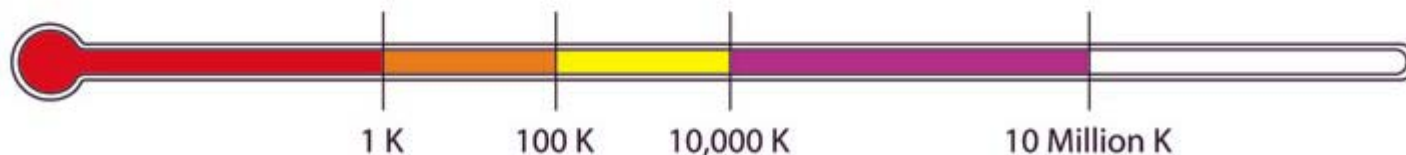
Veliko kao...



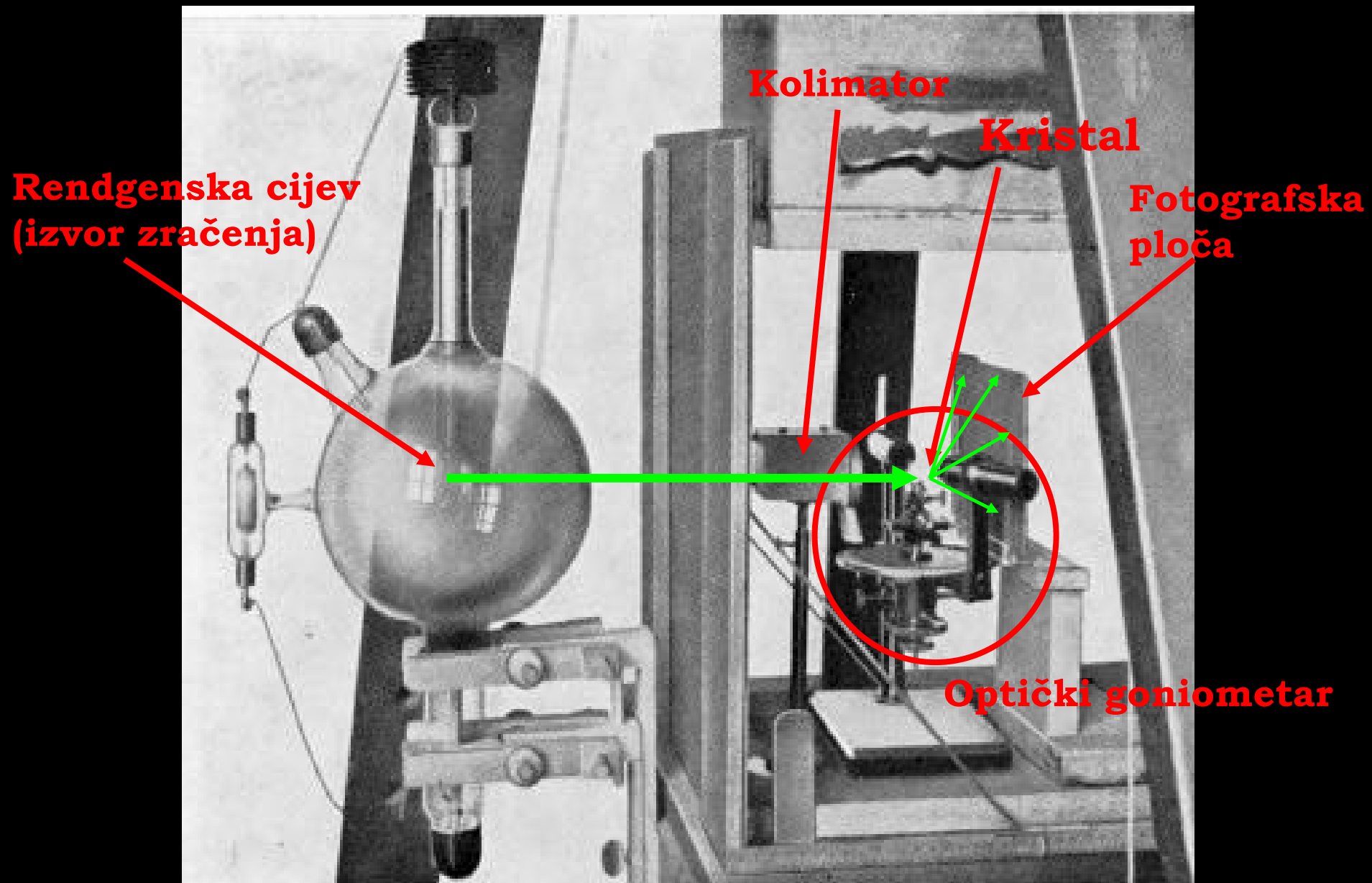
Frekvencija (Hz)



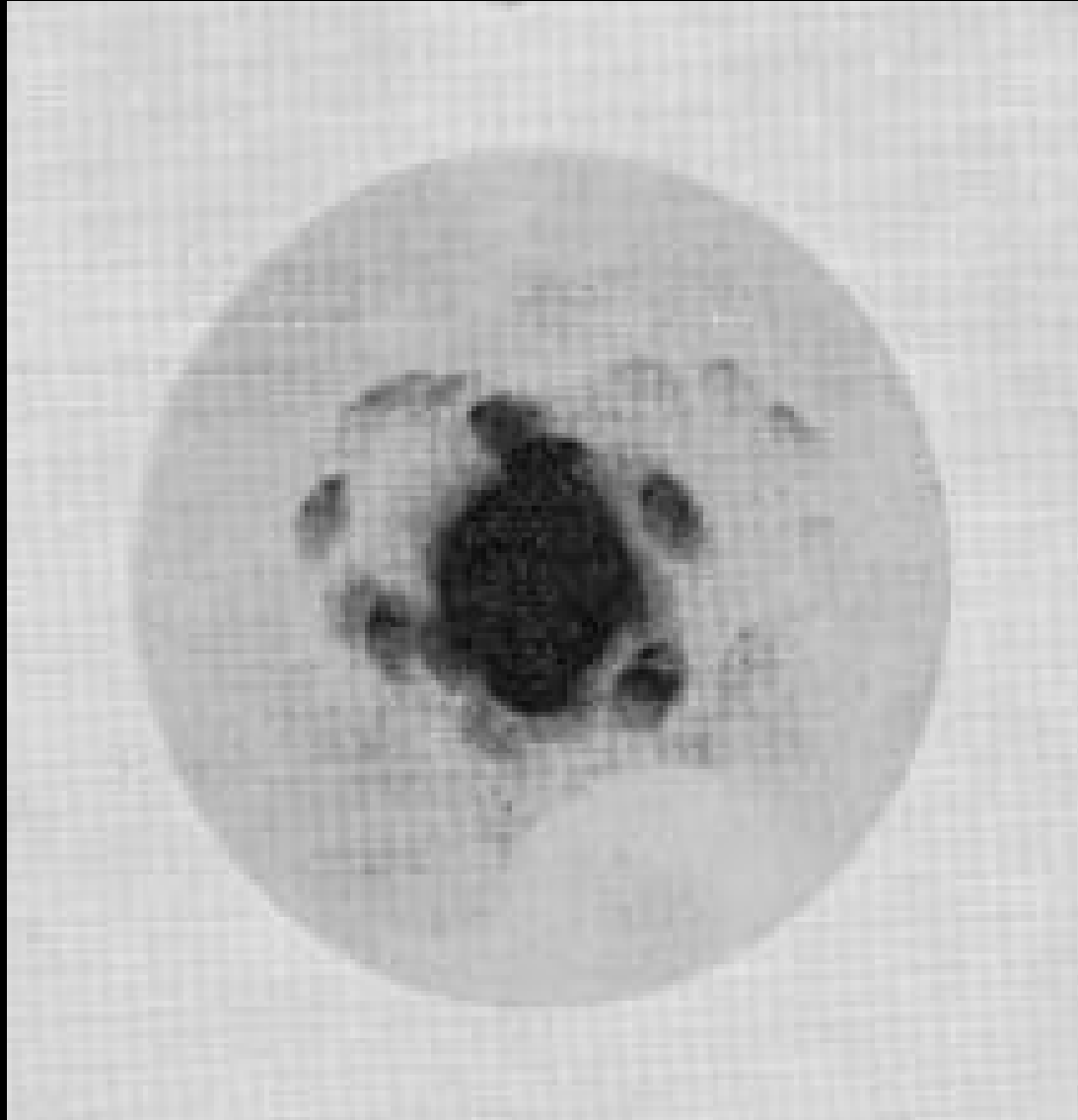
Temperatura (K)



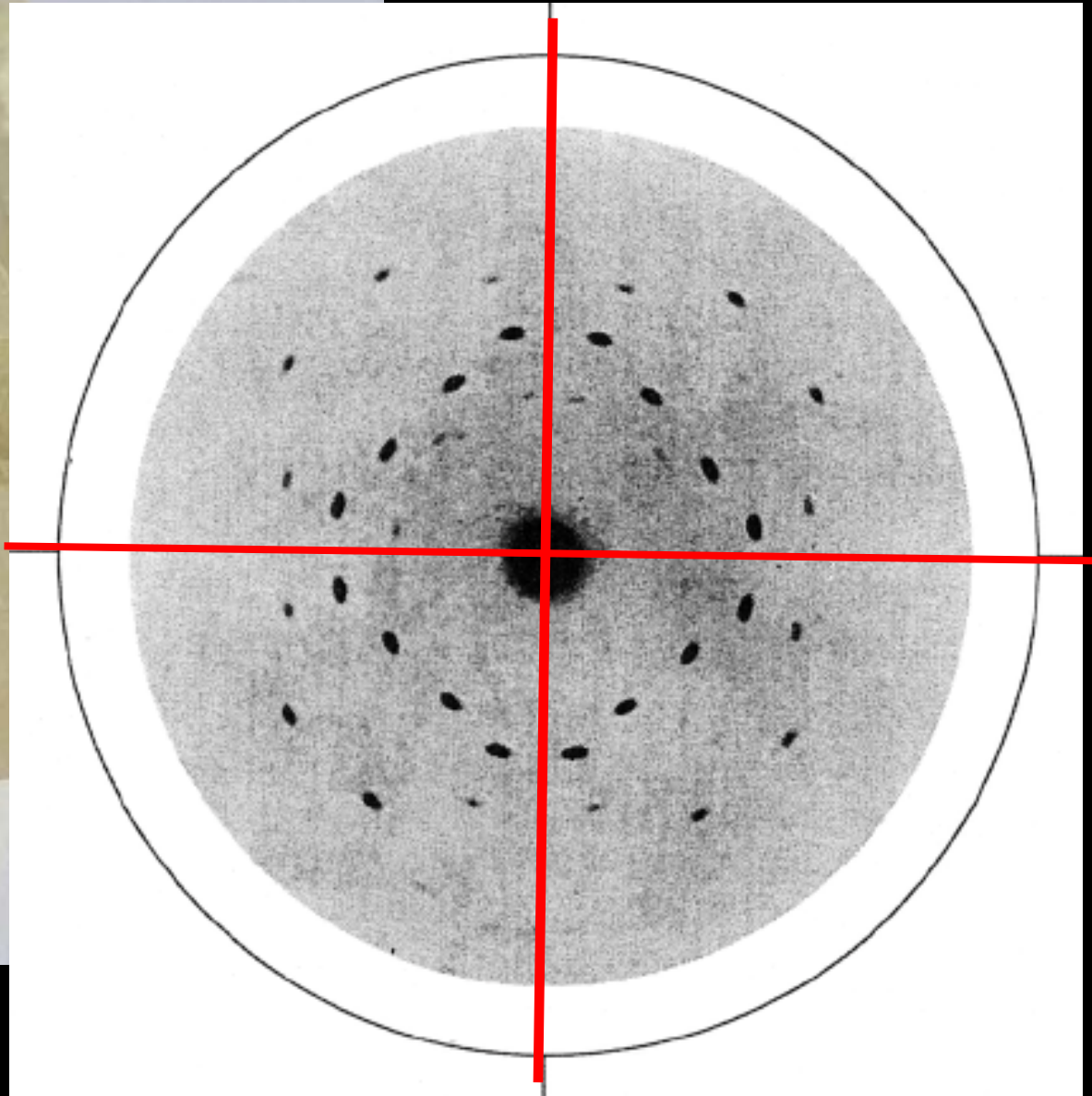
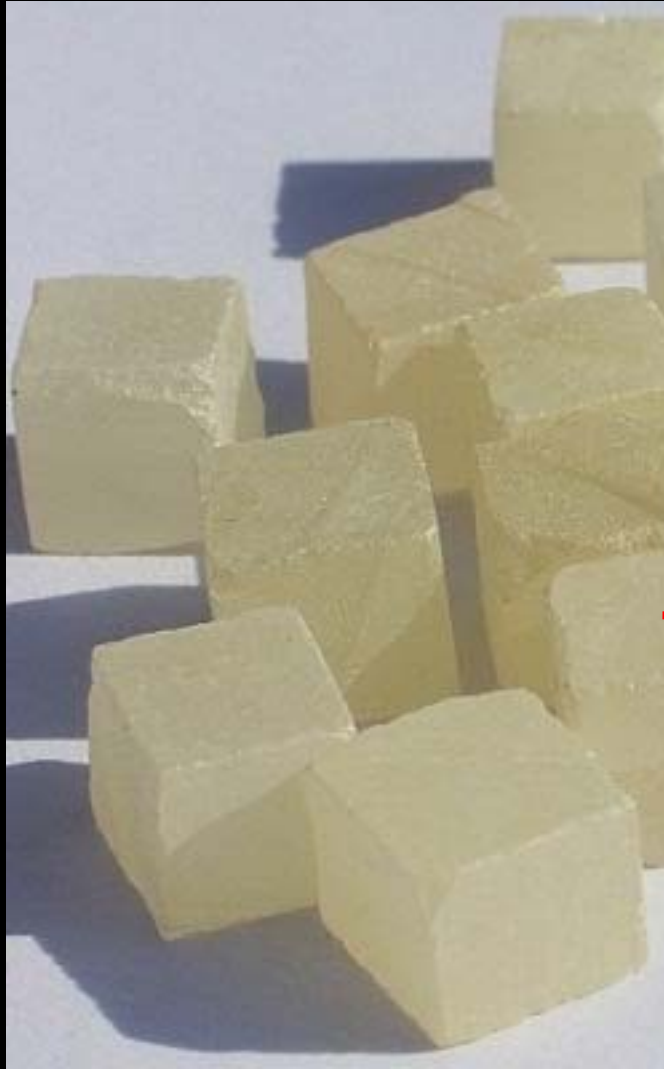
Instrument:



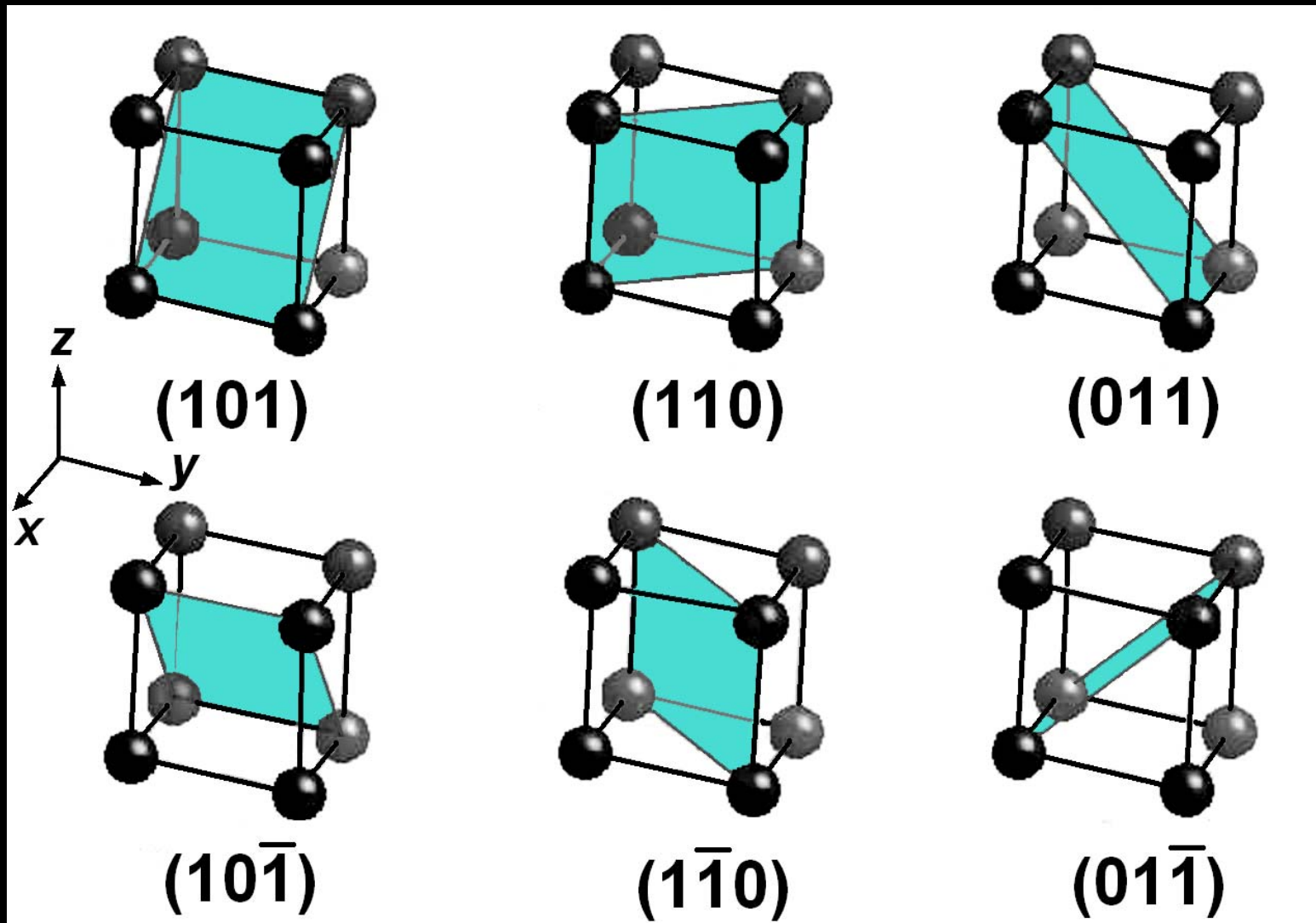
Difrakcija na kristalu modre galice ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$)



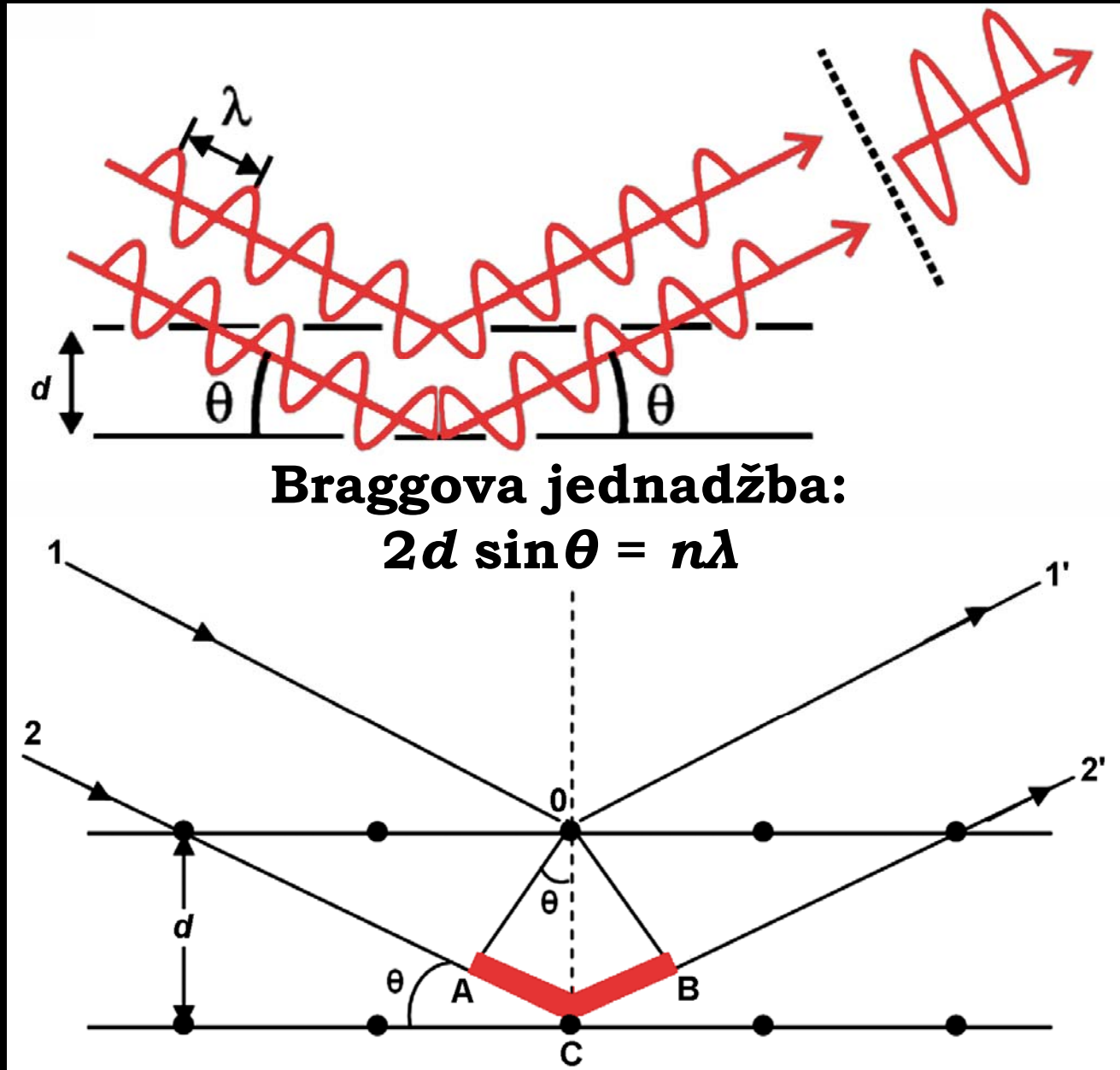
Simetrija u kristalima: ZnS



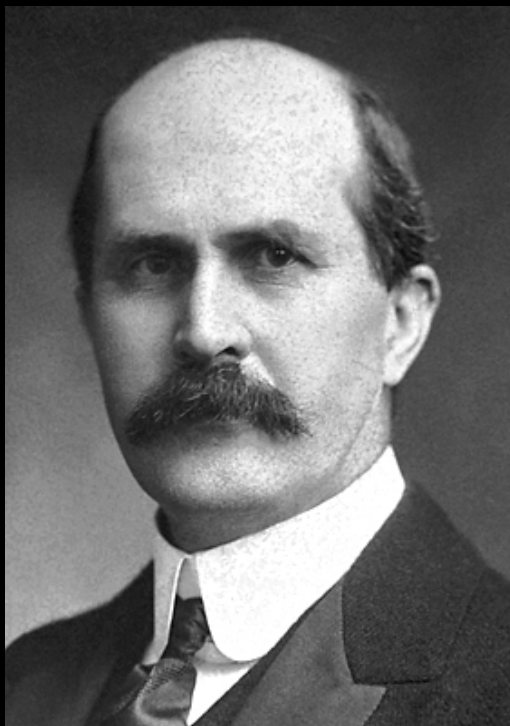
Kristali iznutra: slojevi atoma iliti “mrežne ravnine”



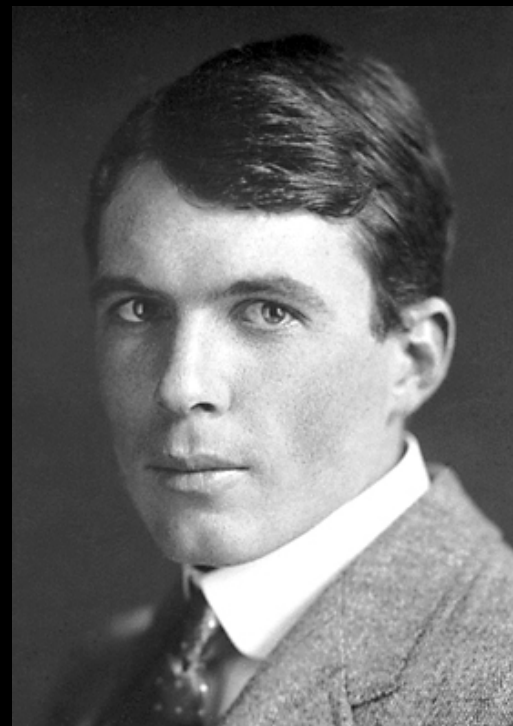
Pojednostavljeno objašnjenje:



Prva kristalna struktura



William Henry Bragg

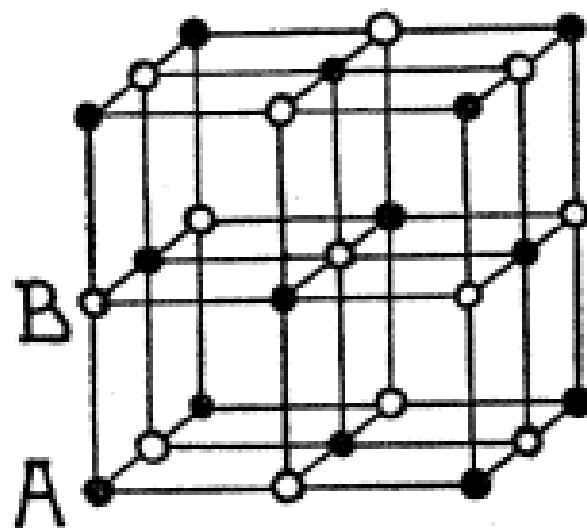
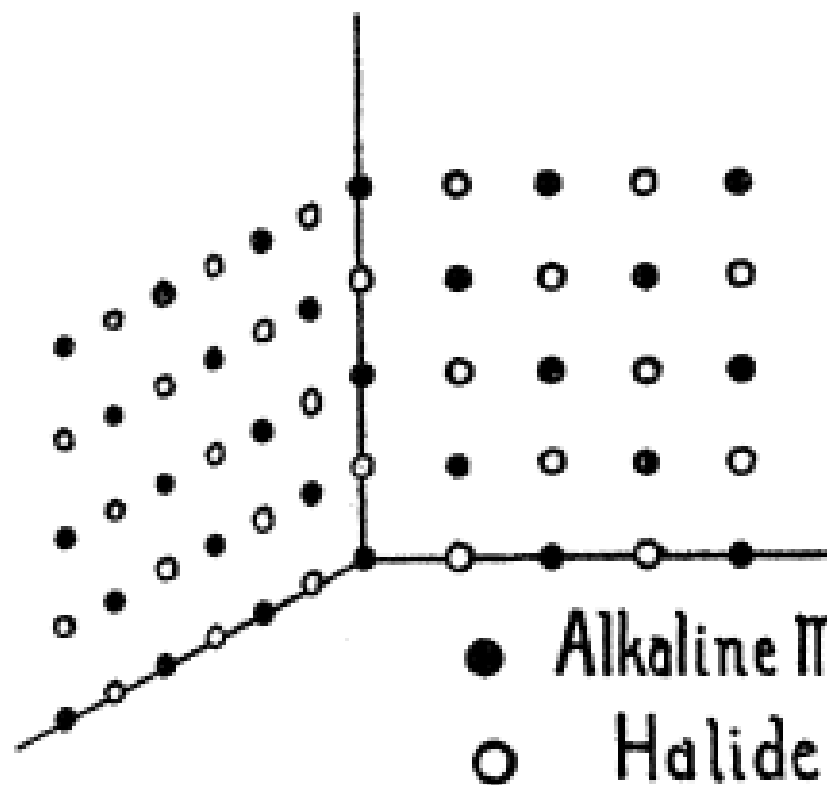


William Lawrence Bragg

NaCl, KCl, KBr i KI, 1913.

Nobelova nagrada 1915.

Natrijev klorid (Braggovi, 1913.)

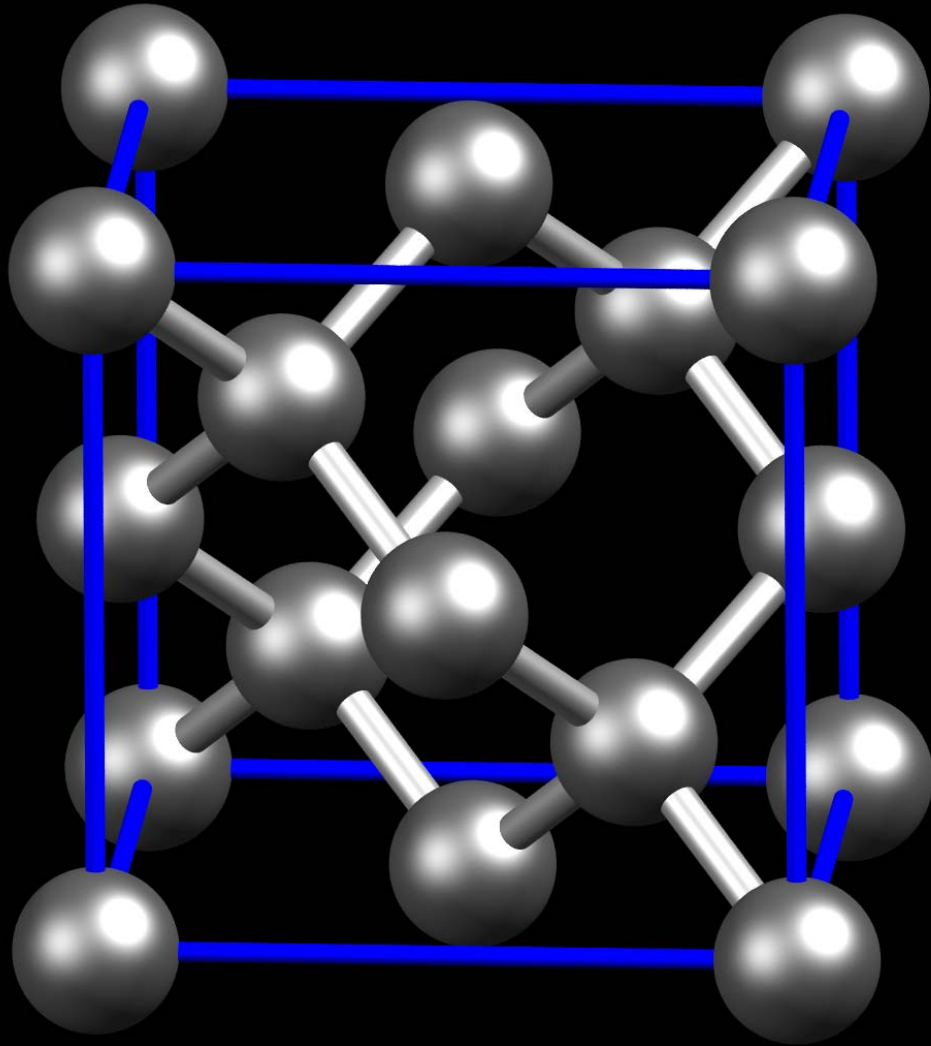


For NaCl

$$AB = 2.8 \cdot 10^{-8} \text{ cm.}$$

FIG. 10.

Dijamant (Braggovi, 1913.)

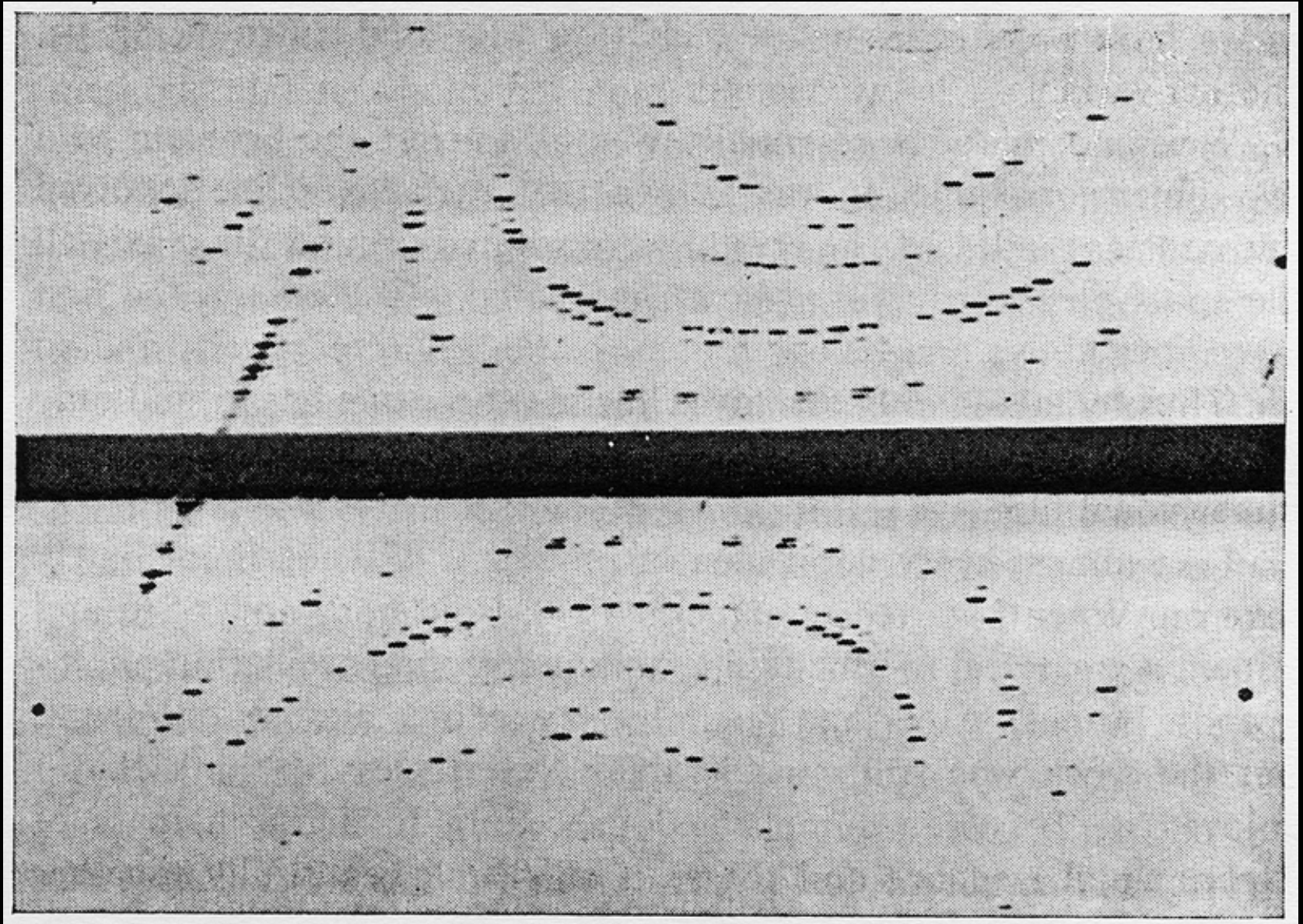


Weissenbergova kamera

(1923.)



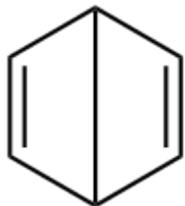
Rendgenske fotografije



Aromatski prsten (K. Lonsdale, 1929.)



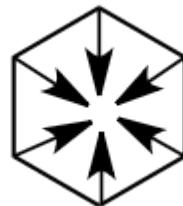
Claus,
1867.



Dewar,
1867.



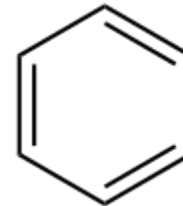
Ladenburg,
1869.



Armstrong,
1889.



Thiele,
1899.



Kekulé,
1865.

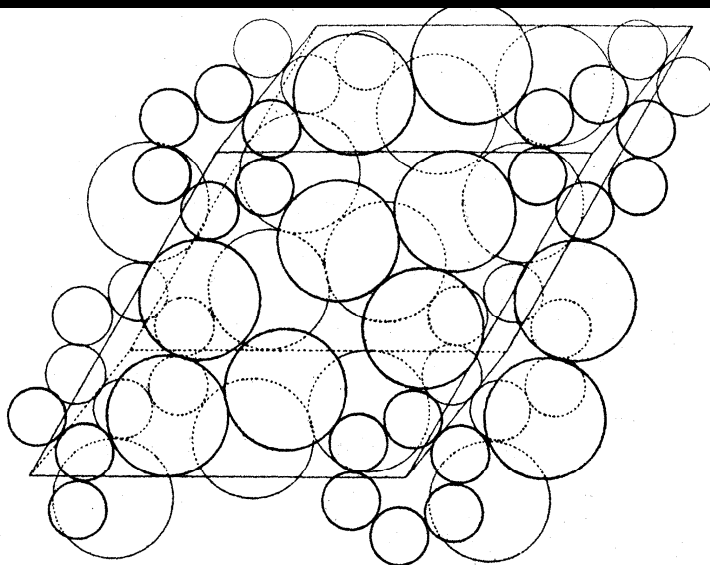
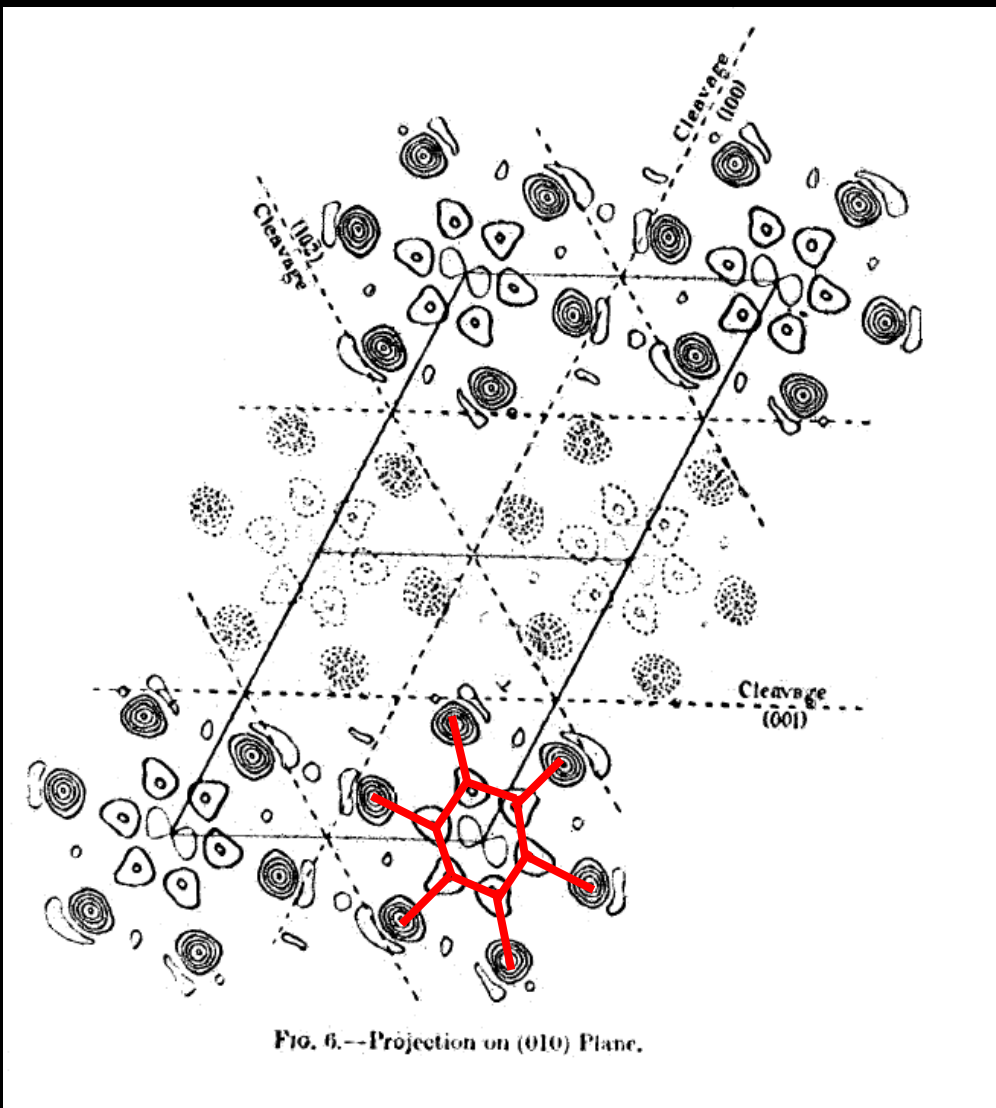
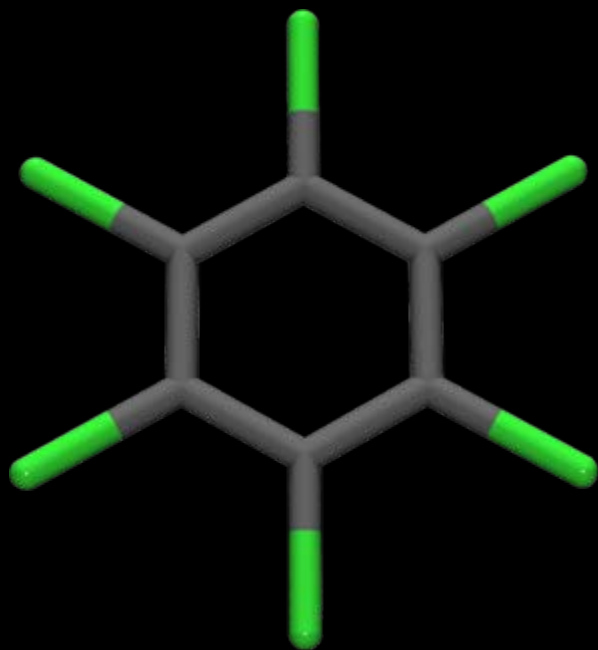


FIG. 14.—Orthogonal projection of unit cell on to (001) plane.

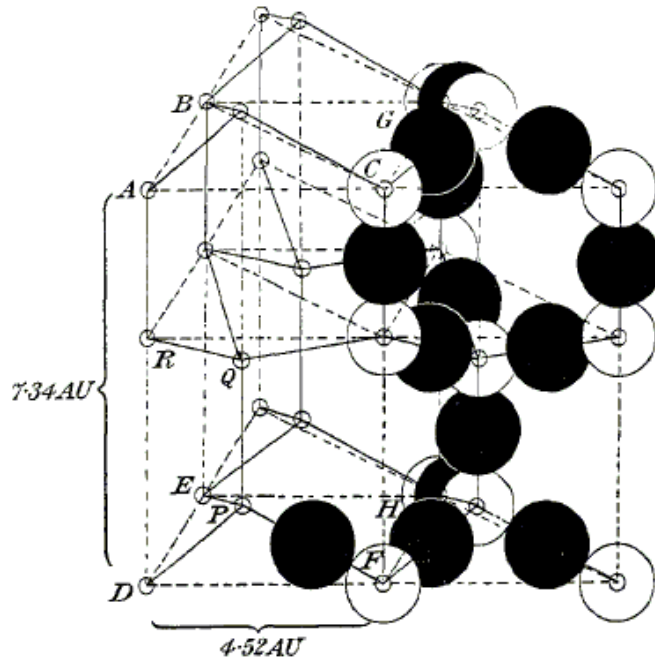
kristali heksametilbenzena

Heksaklorbenzen (K. Lonsdale, 1931.)

Mapa elektronske
gustoće

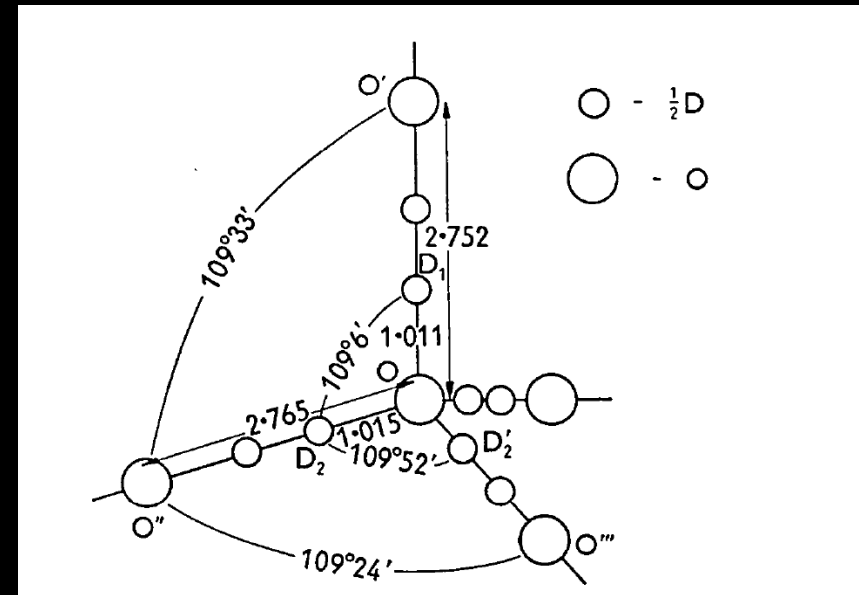


Led (1922. – 1957.)

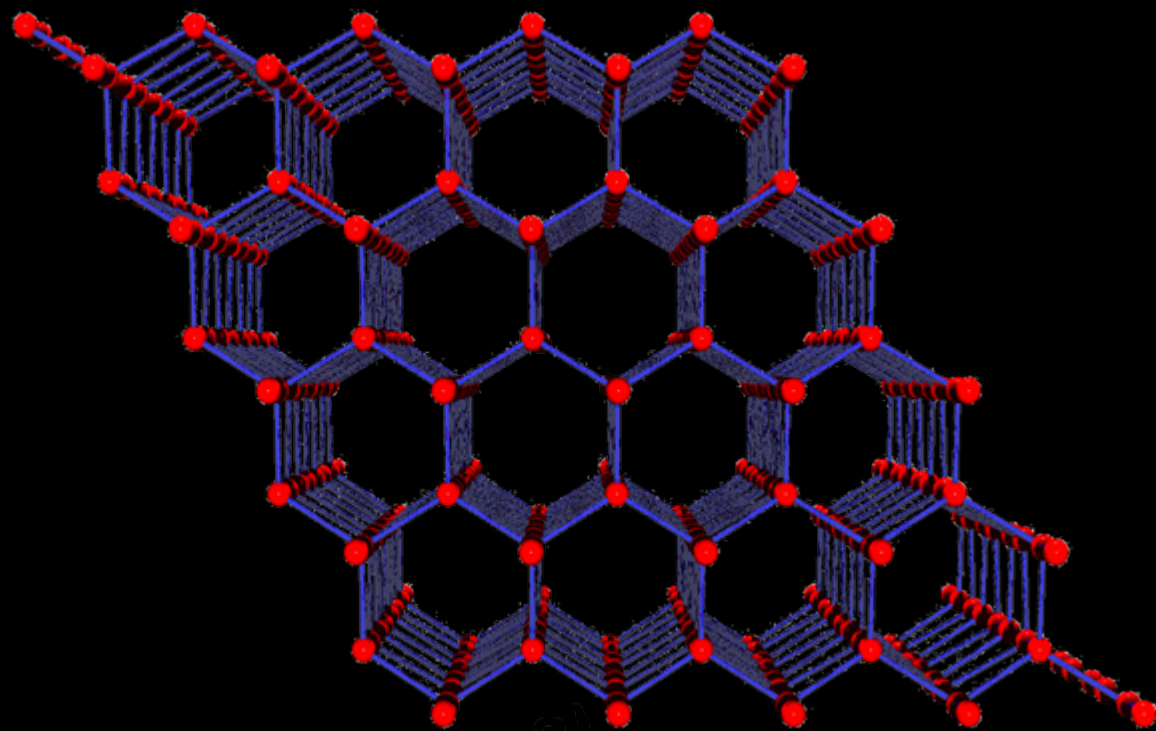
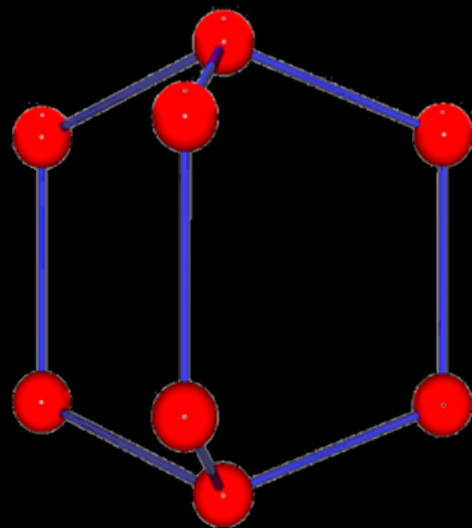
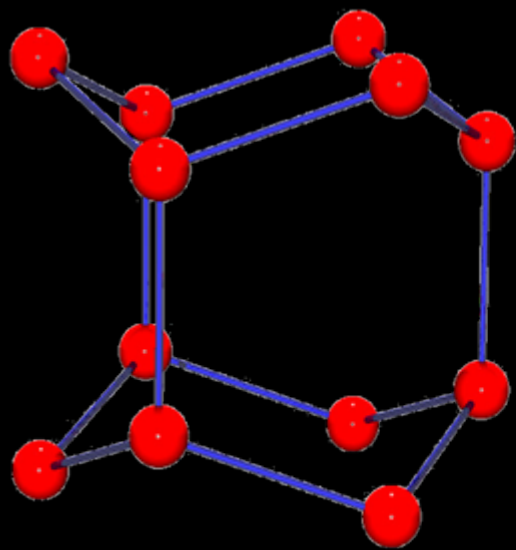


BLACK CIRCLES REPRESENT HYDROGEN ATOMS; WHITE CIRCLES REPRESENT OXYGEN ATOMS.

Bragg, 1922.
Raspored kisikovih atoma

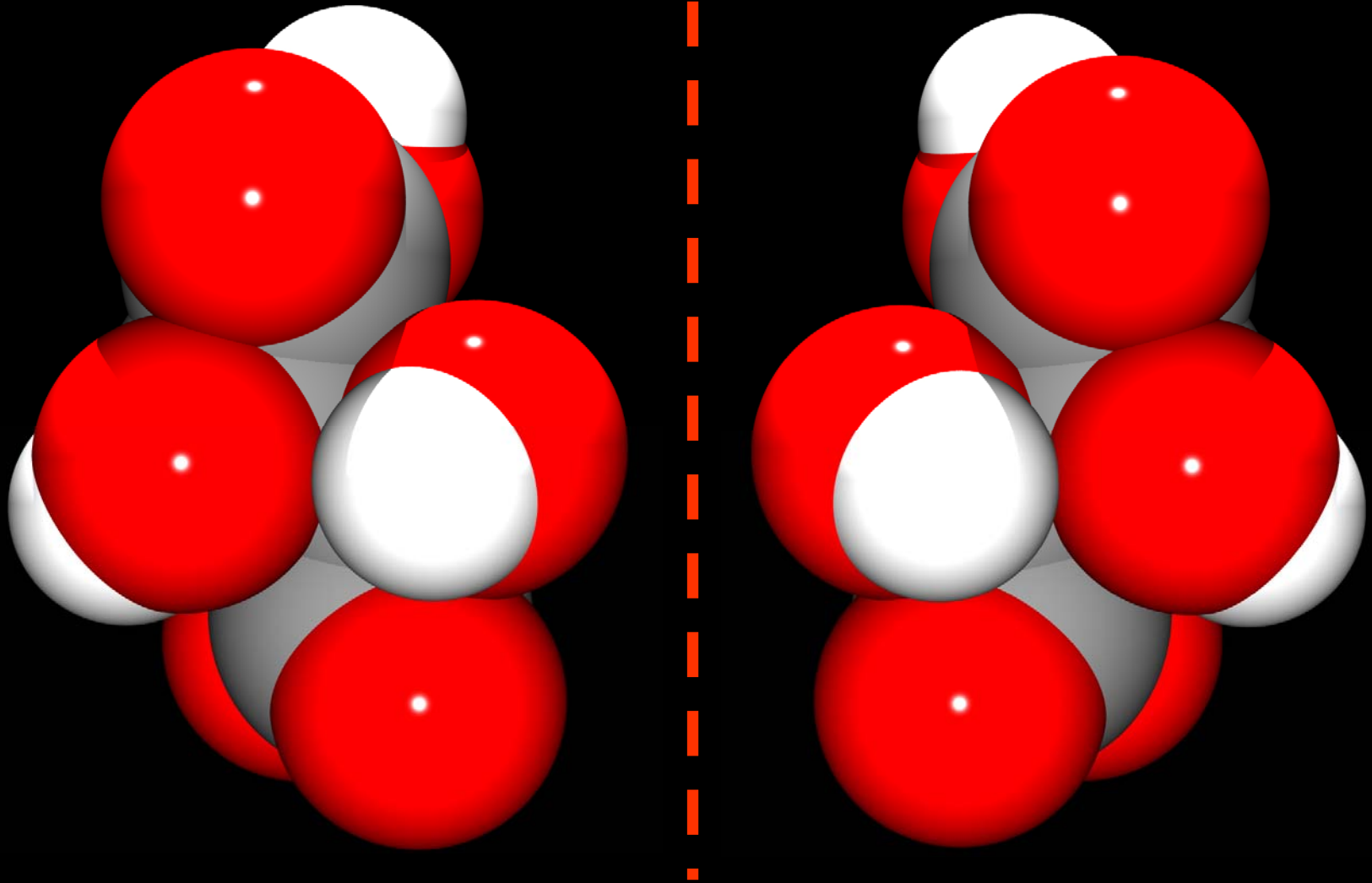


Peterson i Levy, 1957.
Položaji vodikovih atoma,
u neredu



a)

Apsolutna konfiguracija (Bijvoet, 1949.)

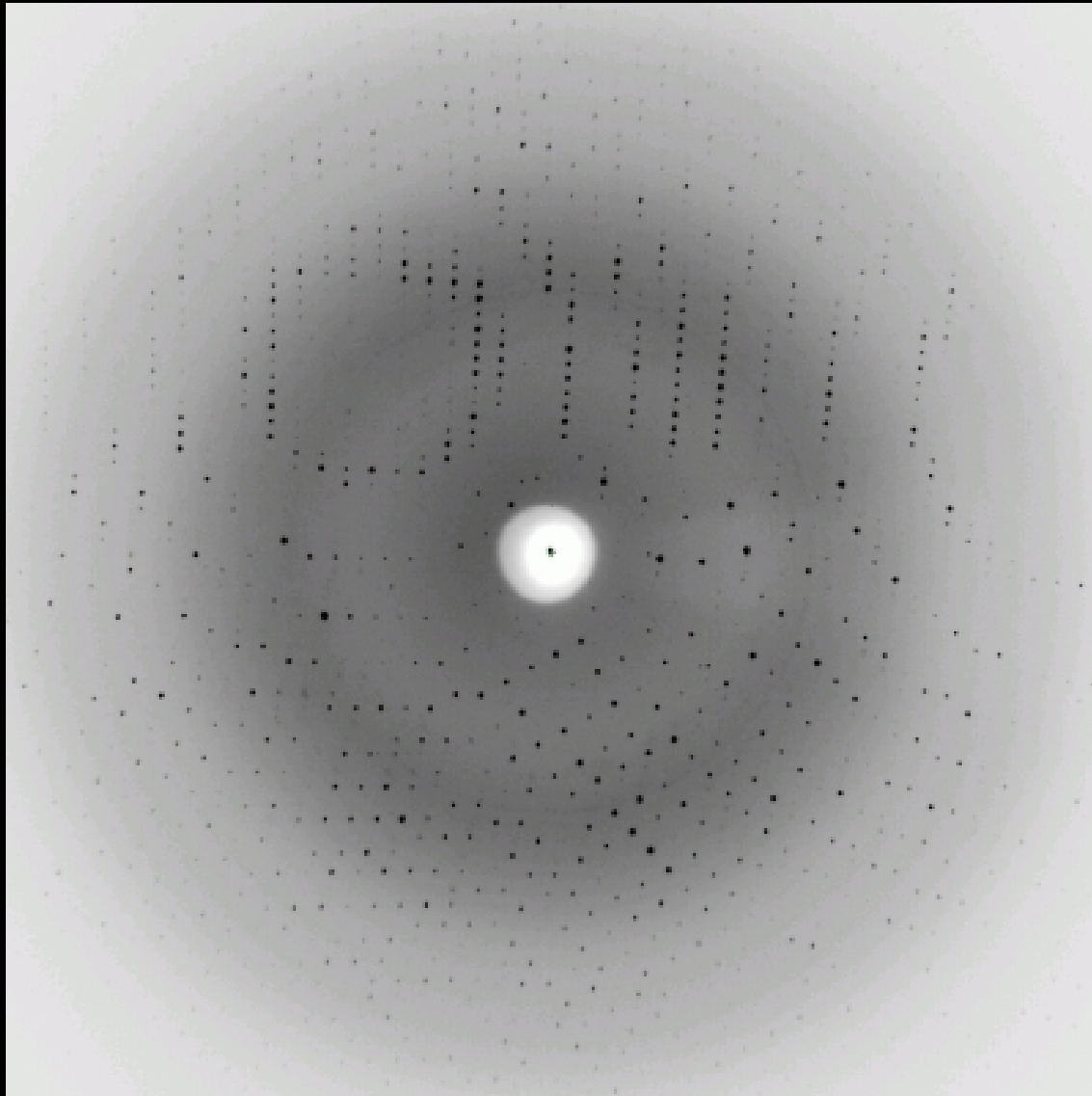


kristali natrijevog rubidijevog tartarata

Automatski difraktometri



Rendgenska “digitalna” fotografija

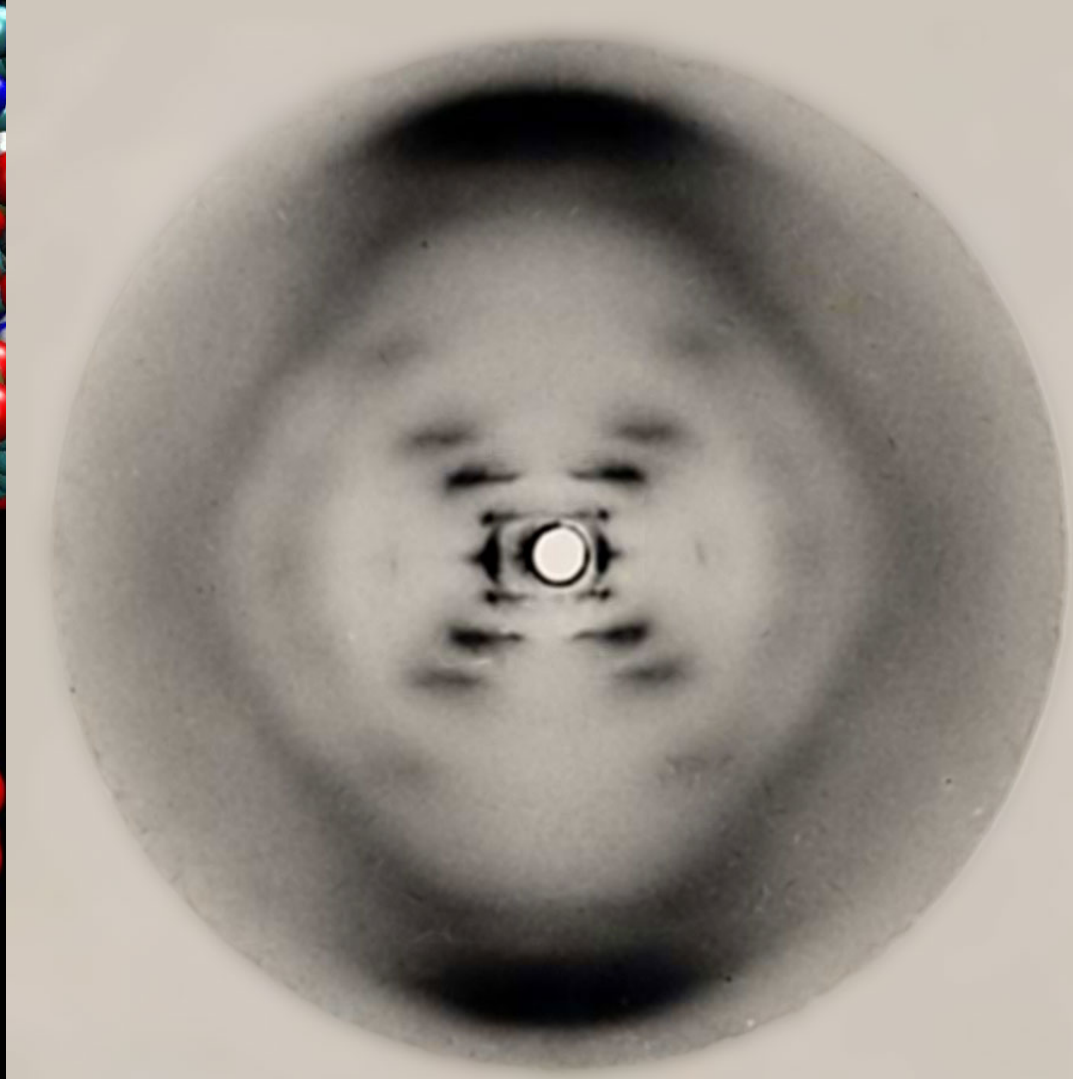
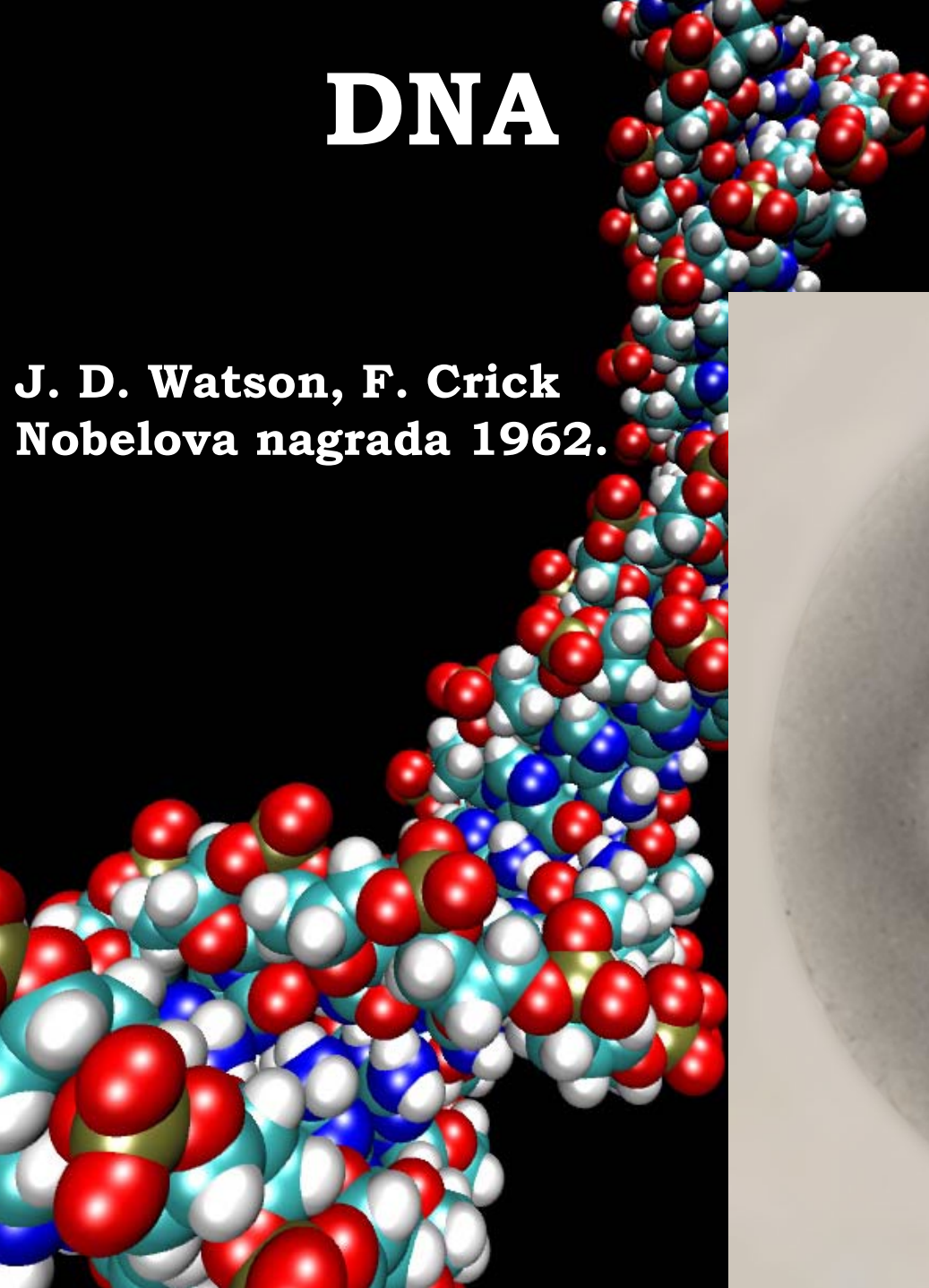


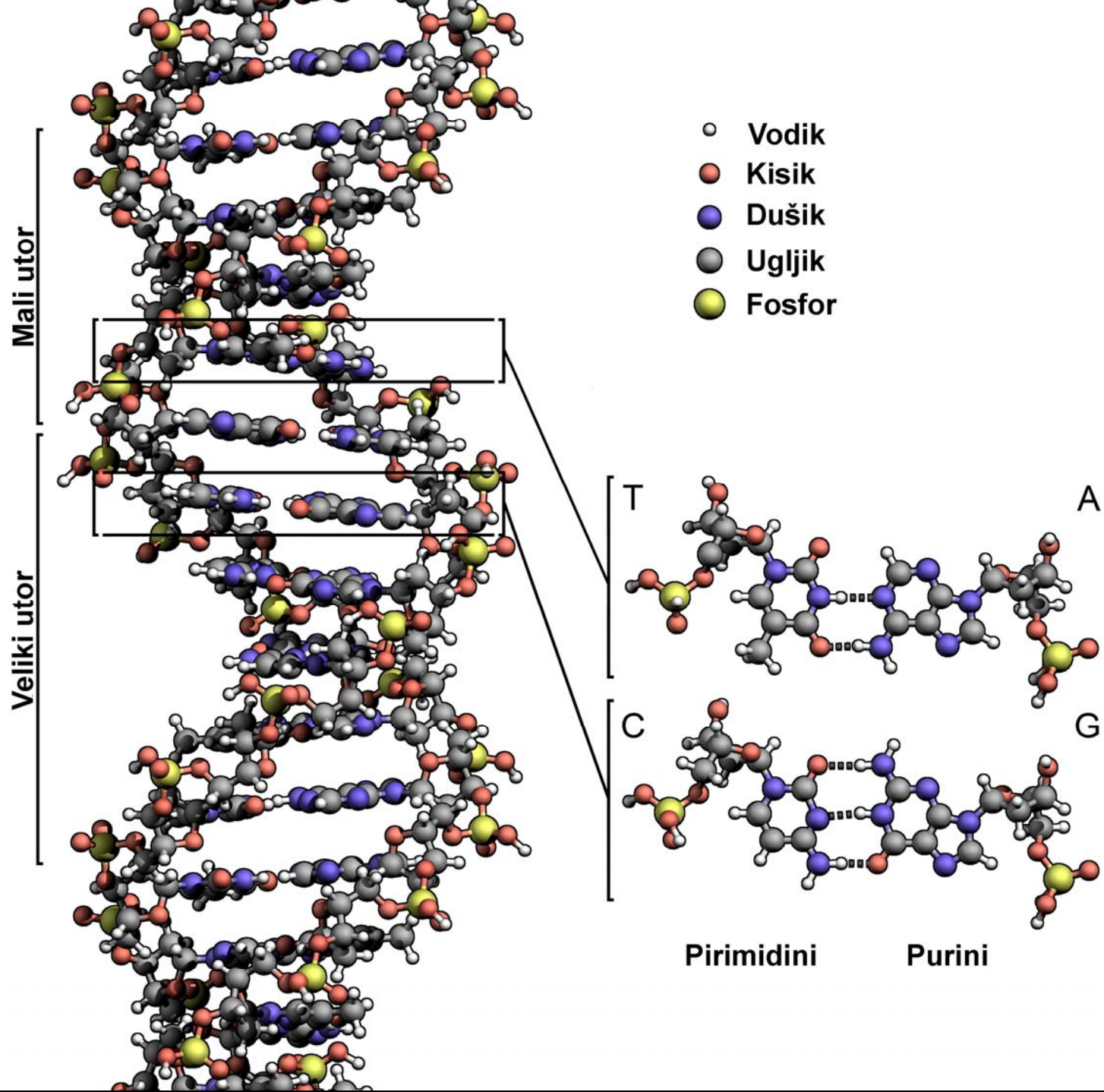
DNA

(1953.)

R. Franklin, M. Wilkins

J. D. Watson, F. Crick
Nobelova nagrada 1962.

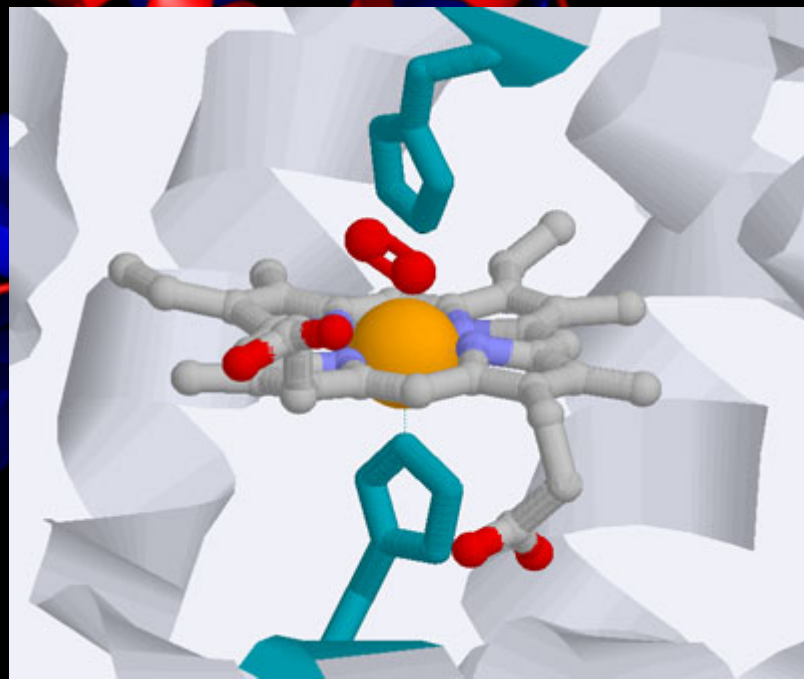
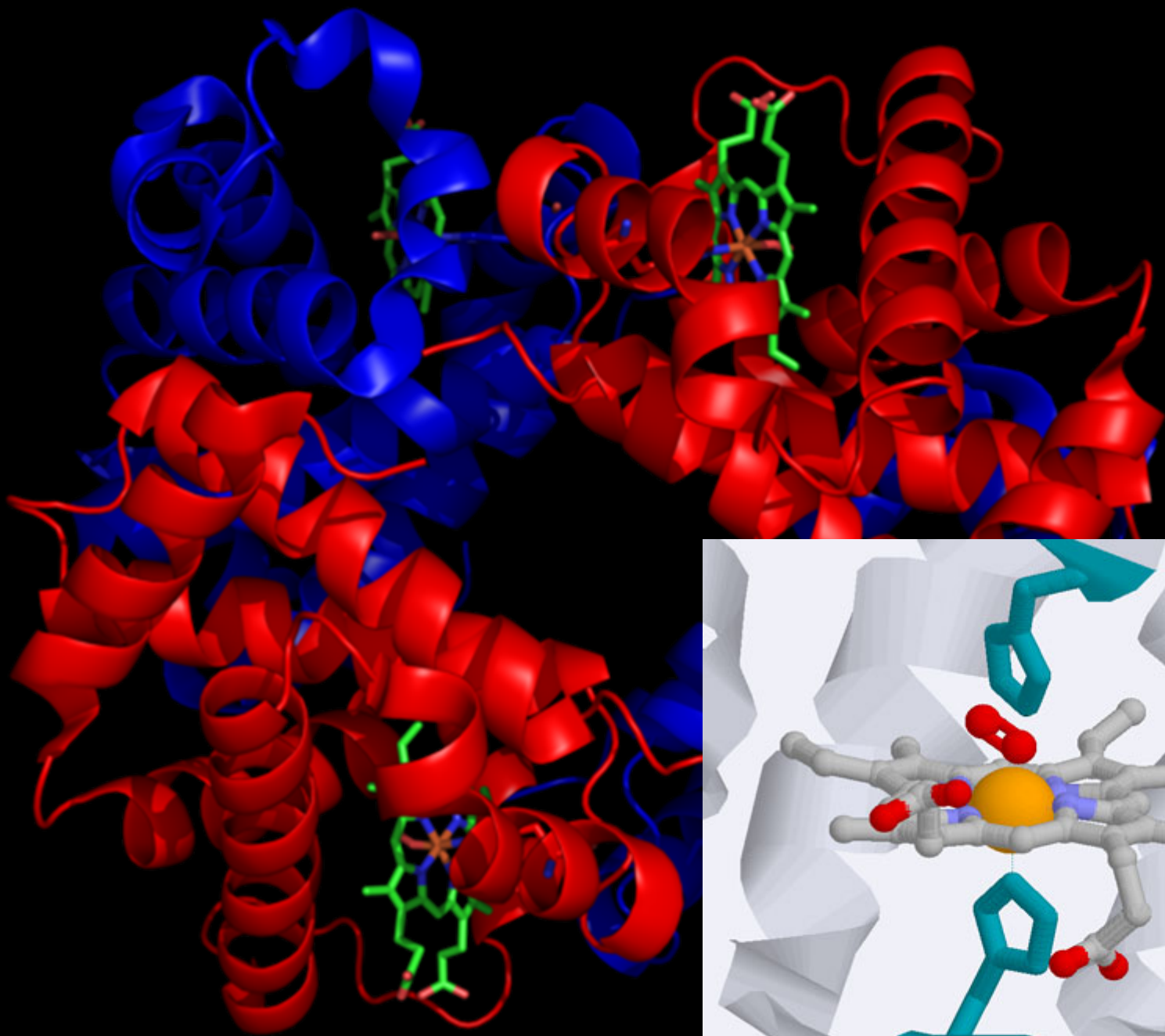




Hemoglobin (M. Perutz, 1959.)



Počeo još 30-ih
Nobelova nagrada 1962.



Sinkrotron (ESRF u Grenobleu)

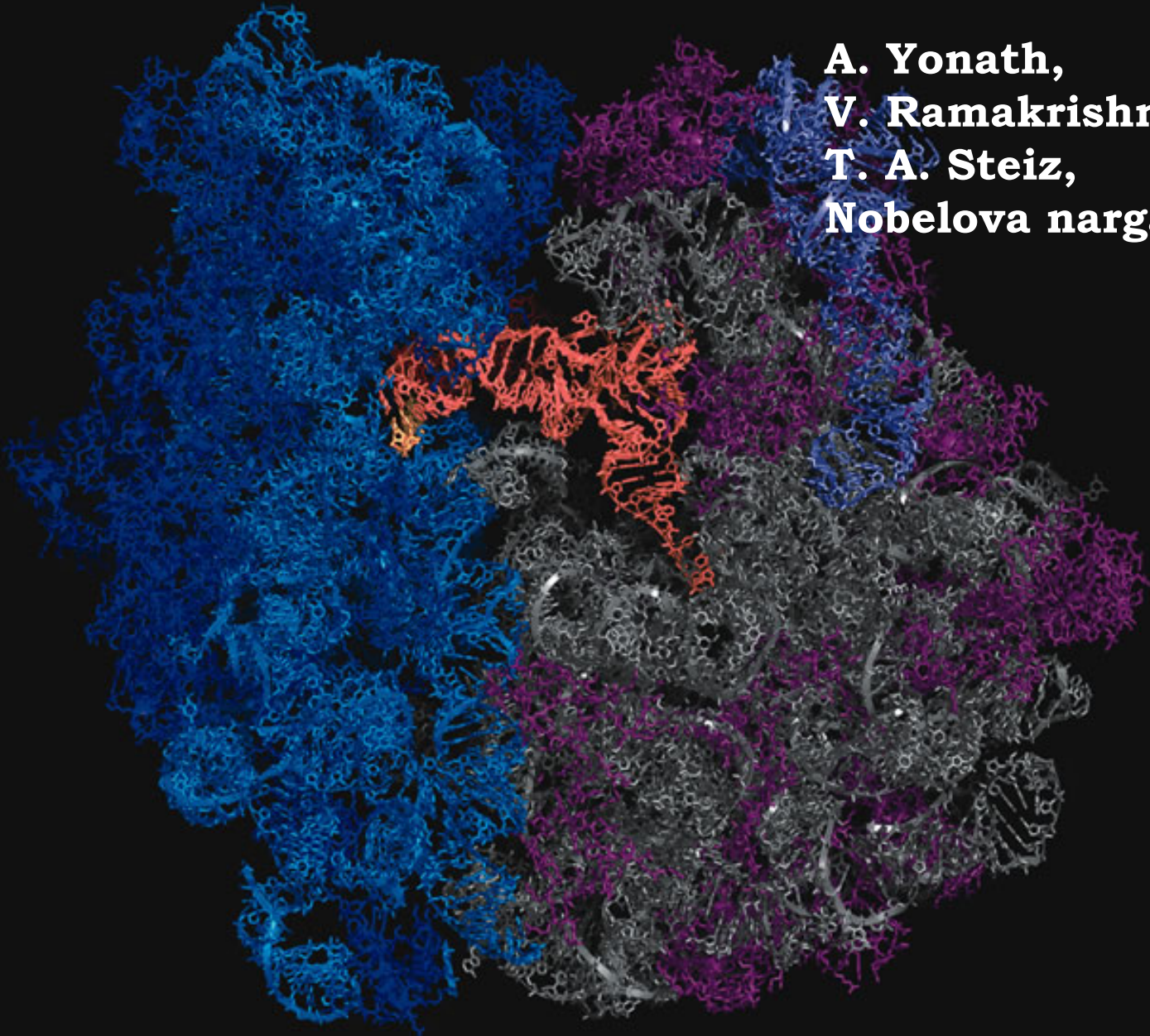




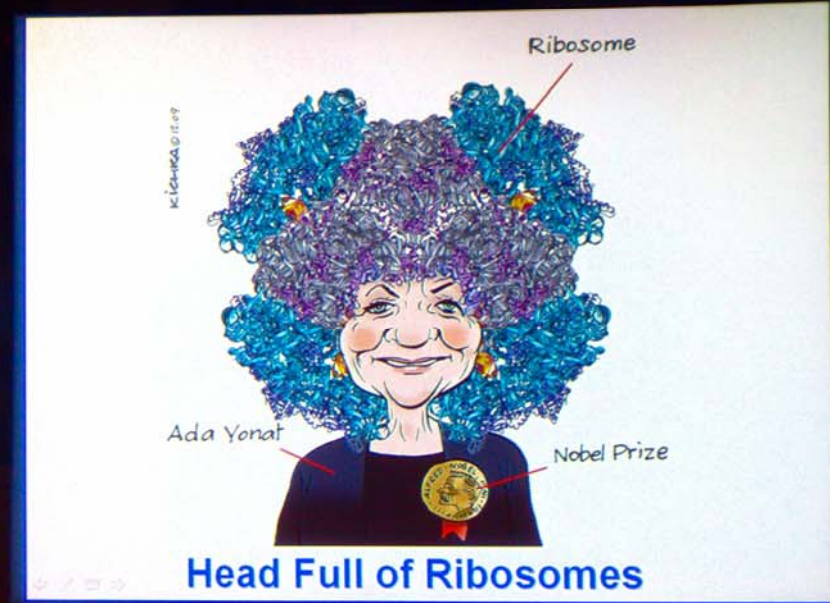


Ribosom (1999./2000.)

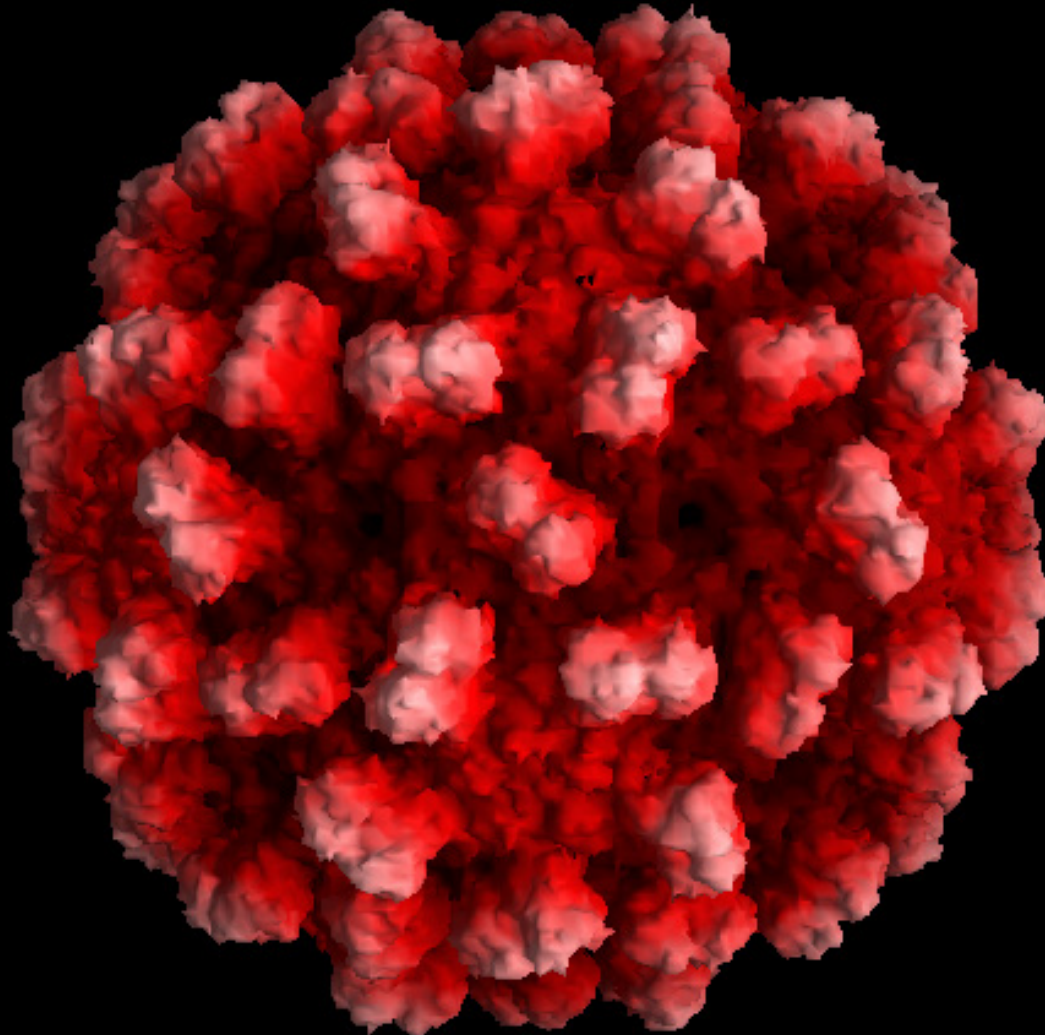
A. Yonath,
V. Ramakrishnan,
T. A. Steiz,
Nobelova nargada 2009.



Ada Yonath (u Madridu, 2011.)



Virus patuljaste nakaznosti rajčice (1978.)



*Tomato
Bushy
stunt
Virus*

*X-ray Structure
determination:*

*S.C. HARRISON, A.J.
OLSON, C.E. SCHUTT, F.K.
WINKLER,
G.BRIC OGNE (1978)
Nature 276 368*

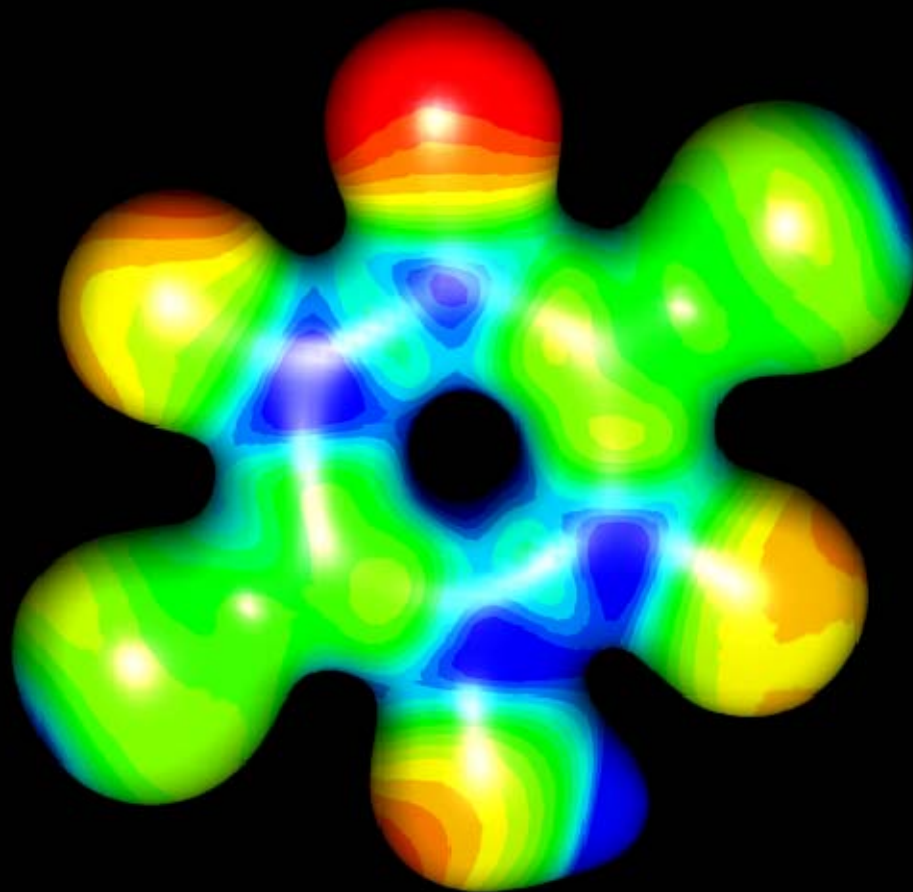
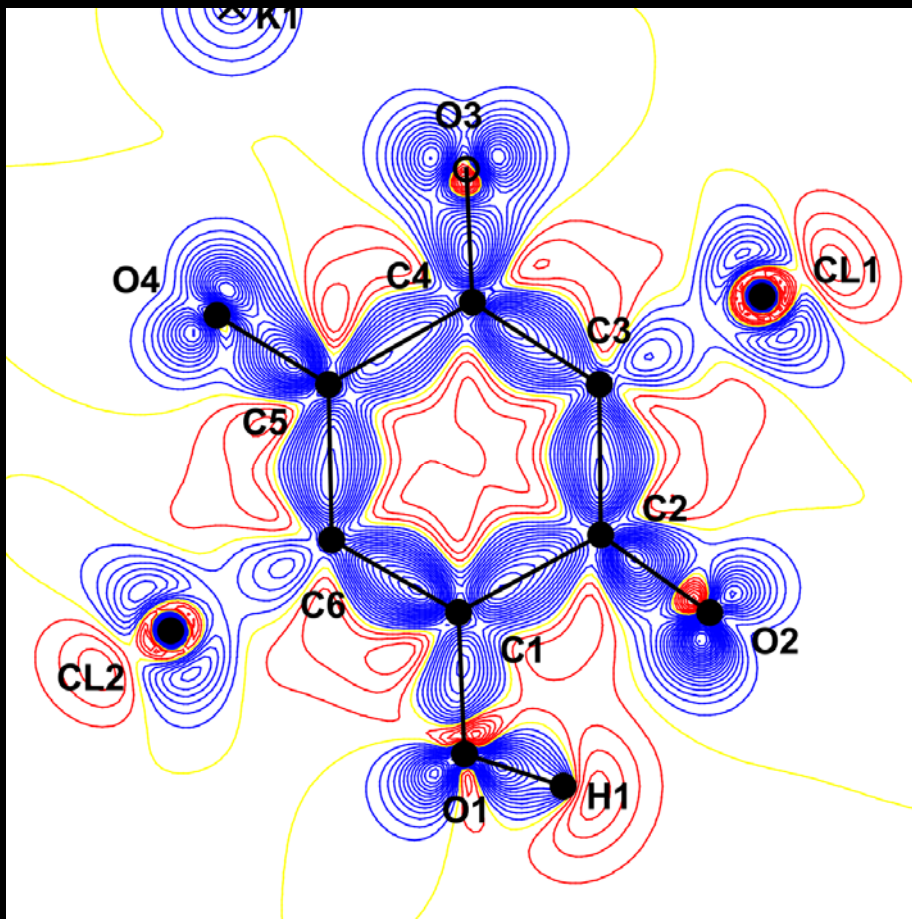
(PDB ENTRY: 2TBV)

*Radial Depth Cue
Rendering with grasp (A.
NICHOLLS) on Silicon
Graphics:*

J-Y. SGRO

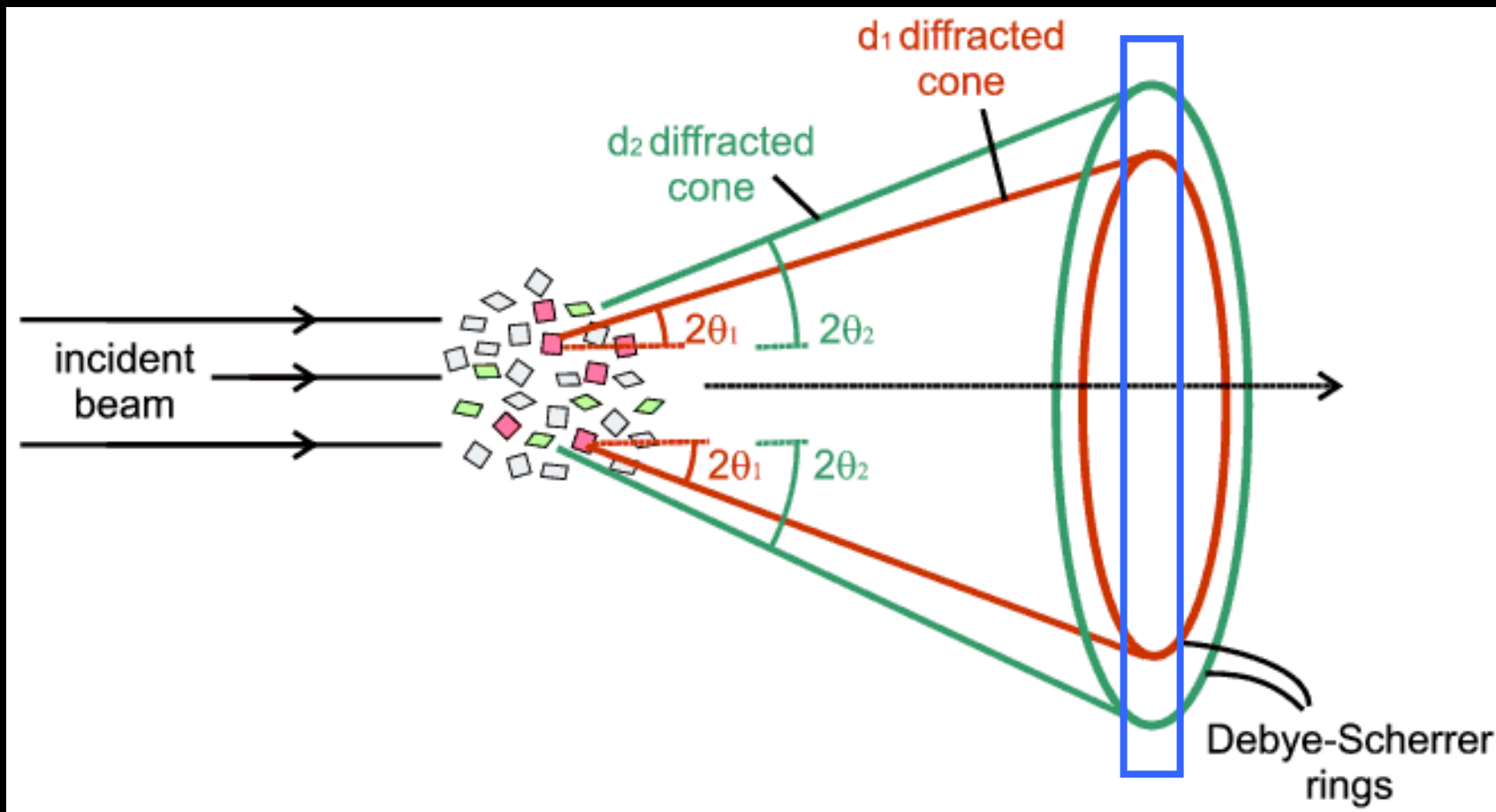
image © 1994 Jean-Yves Sgro

Visoko razlučivanje: raspodjela valentnih elektrona



Difrakcija na prahu

1916./1917. Debye i Scherrer u Njemačkoj, Hull u SAD-u
1969. Rietveld – određivanje strukture iz praha



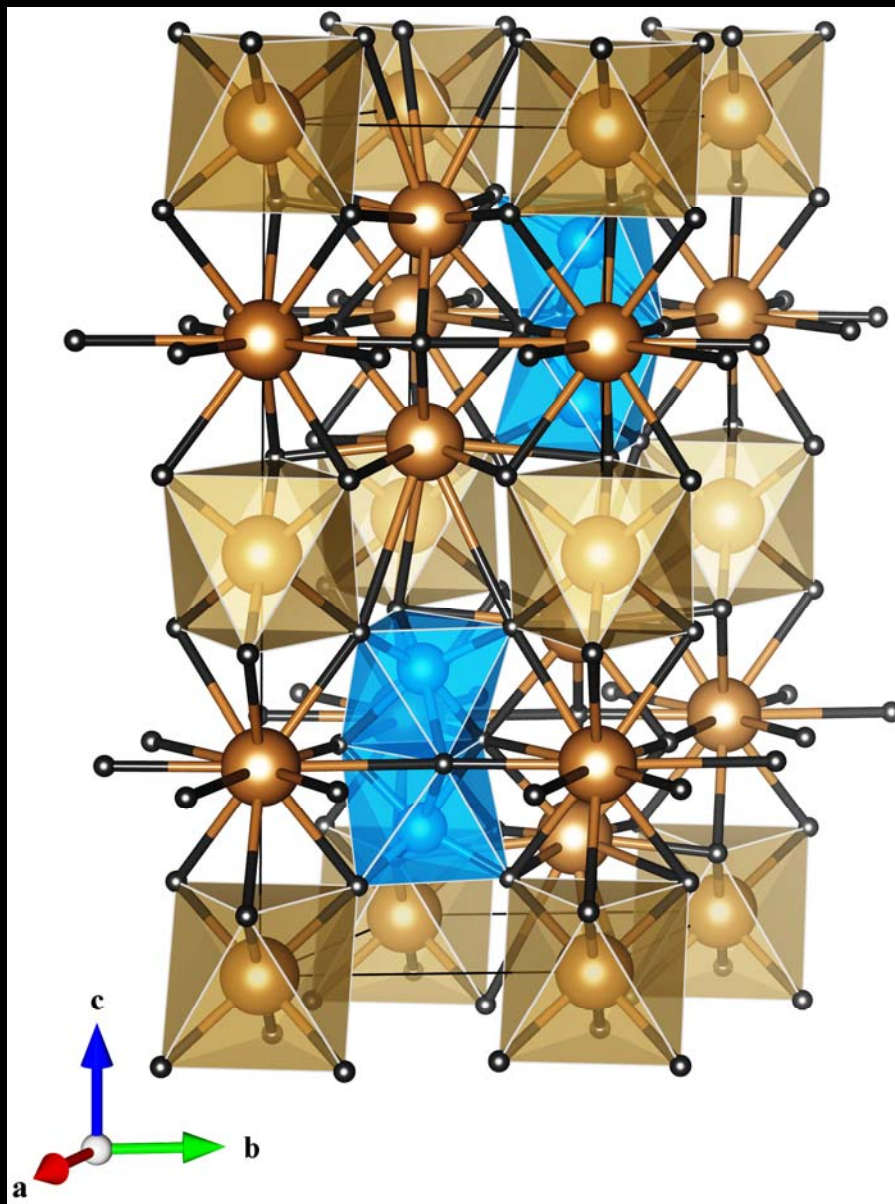
Debye-Scherrerova kamera



Difraktometar za prah



δ -Ba₄Nb₂O₉ iz praha



M. Jurić, J. Popović,
A. Šantić, *Inorg. Chem.*,
2013.

Quo vadis?

- **Poznato je blizu milijun kristalnih struktura:**
 - **700 000 organskih spojeva (CSD)**
 - **160 000 anorganskih spojeva (ISCDB)**
 - **90 000 proteina (PDB)**
 - **6500 oligonukleotida (NDB)**
 - **više tisuća metala i intermetalnih spojeva (CRYSTMET)**
- **Godišnje 50-ak tisuća novih**
- **Do danas: 28 Nobelovih nagrada**

Quo vadis?



- **Fizika** – interakcija materije i zračenja, raspršenje...
- **Mineralogija** – struktura minerala, sastav stijena
- **Kemija** – 3D građa molekule, stereokemija, međumolekulske interakcije, fini detalji elektronske strukture, dinamika u kristalima...
- **Biologija** – 3D građa bioloških makromolekula, mehanizmi enzimske katalize...
- **Znanost o materijalima** – struktura i sastav materijala, naprezanja u kristalnoj rešetci (stress/strain)...
- **Matematika** – teorija grupa, teorija grafova, kvaziperiodička simetrija...