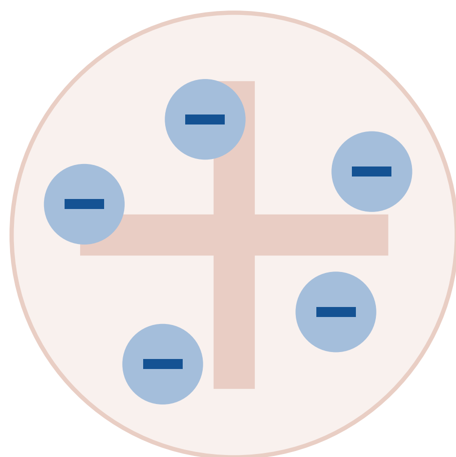
Nuclear Structure and Isomerism

Ian Perry
MacMillan Group Literature Talk
April 29th, 2020

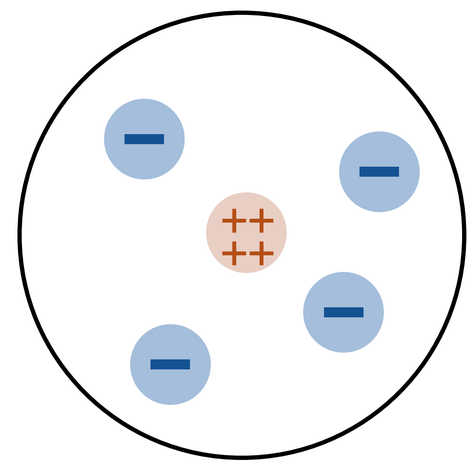
History of Atomic Structure



Thomson Model - 1904

"Plum pudding" – A positive volume filled with negatively charged electrons.

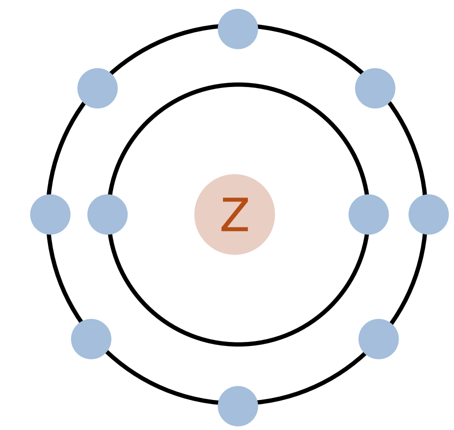
Used to rationalize the apparent negative charge of electrons with the neutrality of free atoms



Rutherford Model - 1911

An area of high positive charge density surrounded by electrons

The Geiger-Marsden Experiment (1909) suggested an area of especially high density within the atom, Rutherford then developed this Nuclear Model

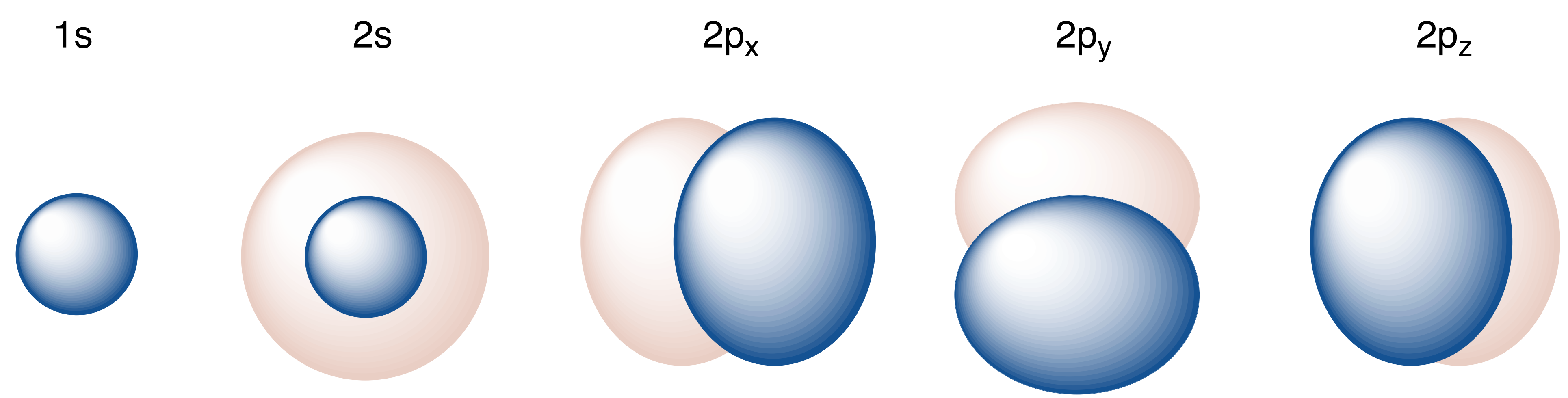


Bohr Model - 1913

Electrons orbiting a nucleus in discrete, well-defined orbits

While more accurate than previous models, physicist couldn't rationalize why electron orbits wouldn't decay

History of Atomic Structure

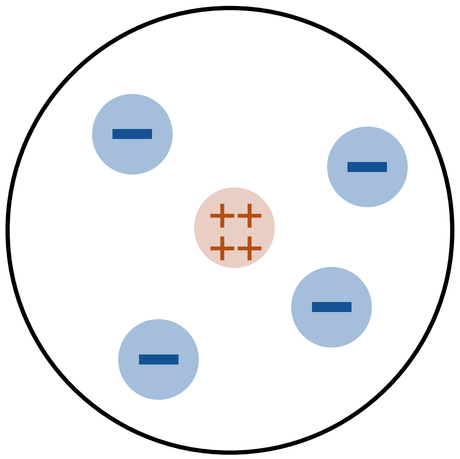


The Quantum Mechanical Model

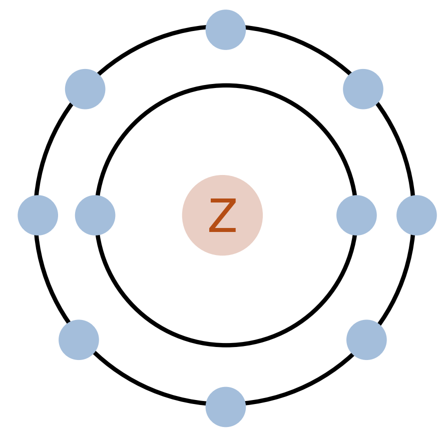
Discrete shells of electrons, with behavior defined by quantum numbers

In chemistry, we traditionally learn about the history of the model of the atom, but rarely cover the model of the nucleus!

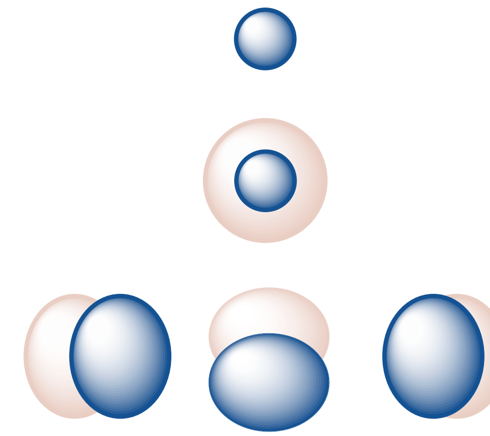
The Nuclear Model



Rutherford

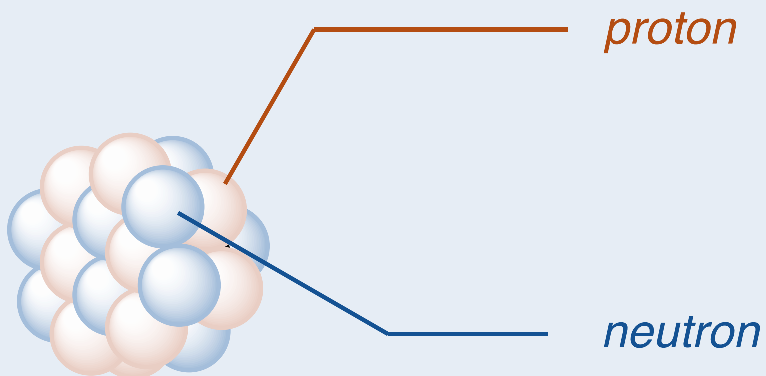


Bohr



Quantum Mechanical

changes in how we think about electron configuration, and thus chemical reactivity



The Nucleus

What dictates nuclear structure?

How does nuclear structure vary between atoms?
Between isotopes? Between Isomers?

What makes a stable nucleus?

Talk Outline

Brief Review of the Atomic Model

Brief Overview: The Standard Model of Particle Physics

The Strong and Residual Strong Interactions

The Nuclear Shell Model

by analogy to the atomic shell model

Nuclear Isomers

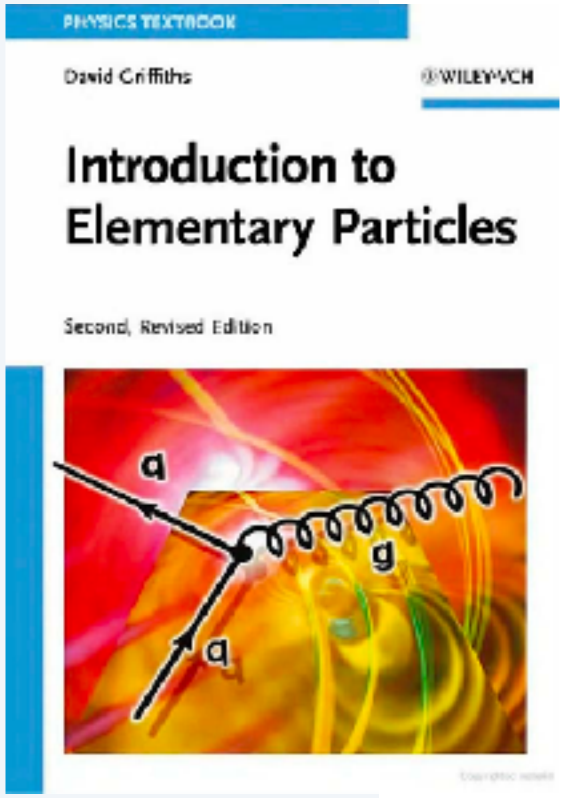
case studies:

^{80m}Br

^{180m}Ta

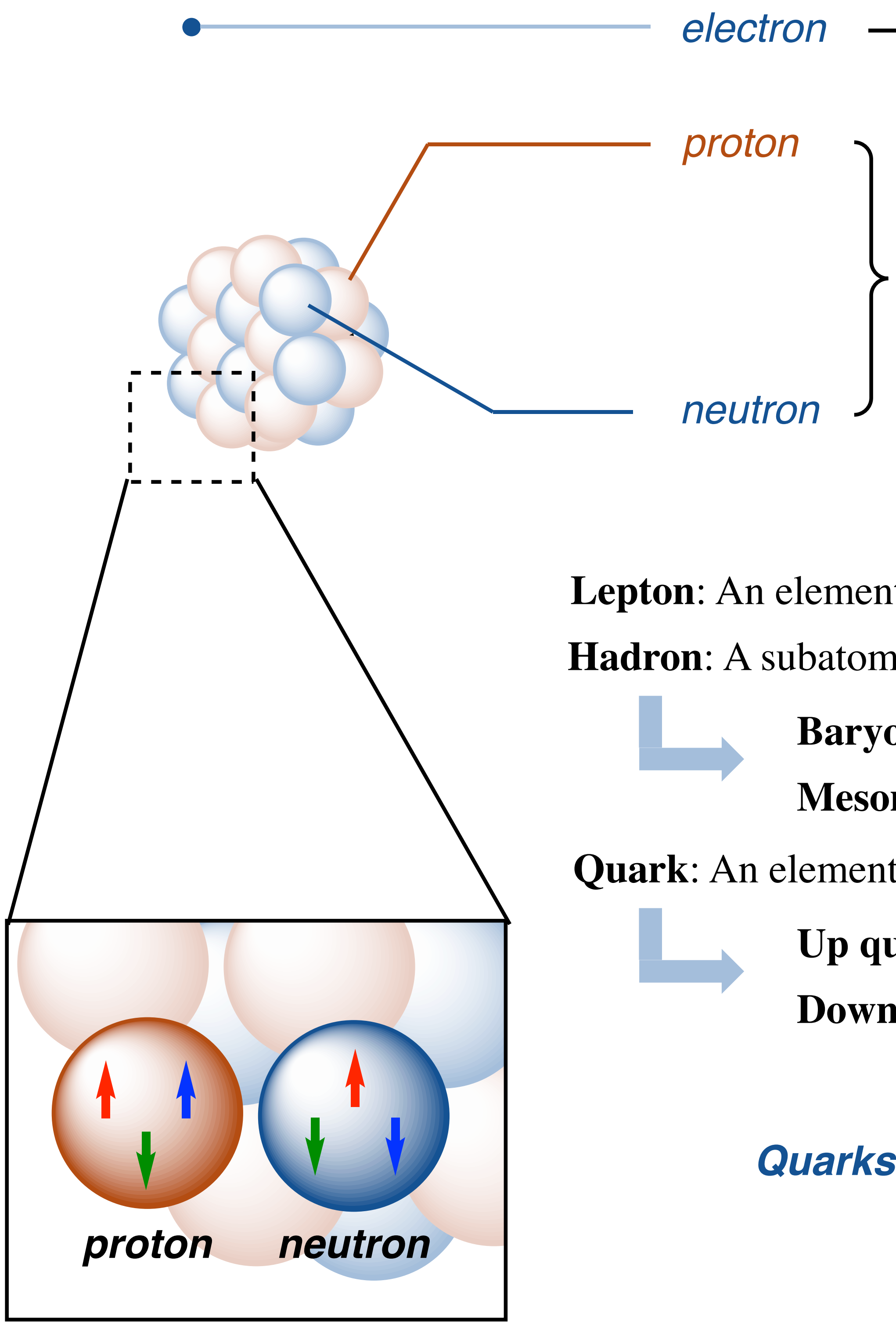
^{99m}Tc

^{229m}Th



Griffiths, D. *Introduction to Elementary Particles, 2nd Ed.;* Wiley, New York, 1987

The Standard Model - An Overview



— elementary particle (lepton)

not elementary particles! (hadron - baryon)

Lepton: An elementary particle of half integer spin that does not undergo strong interactions

Hadron: A subatomic particle comprised of two or more quarks

- **Baryon**: A hadron made up of an odd number of quarks
- **Meson**: A hadron made up of an even number of quarks

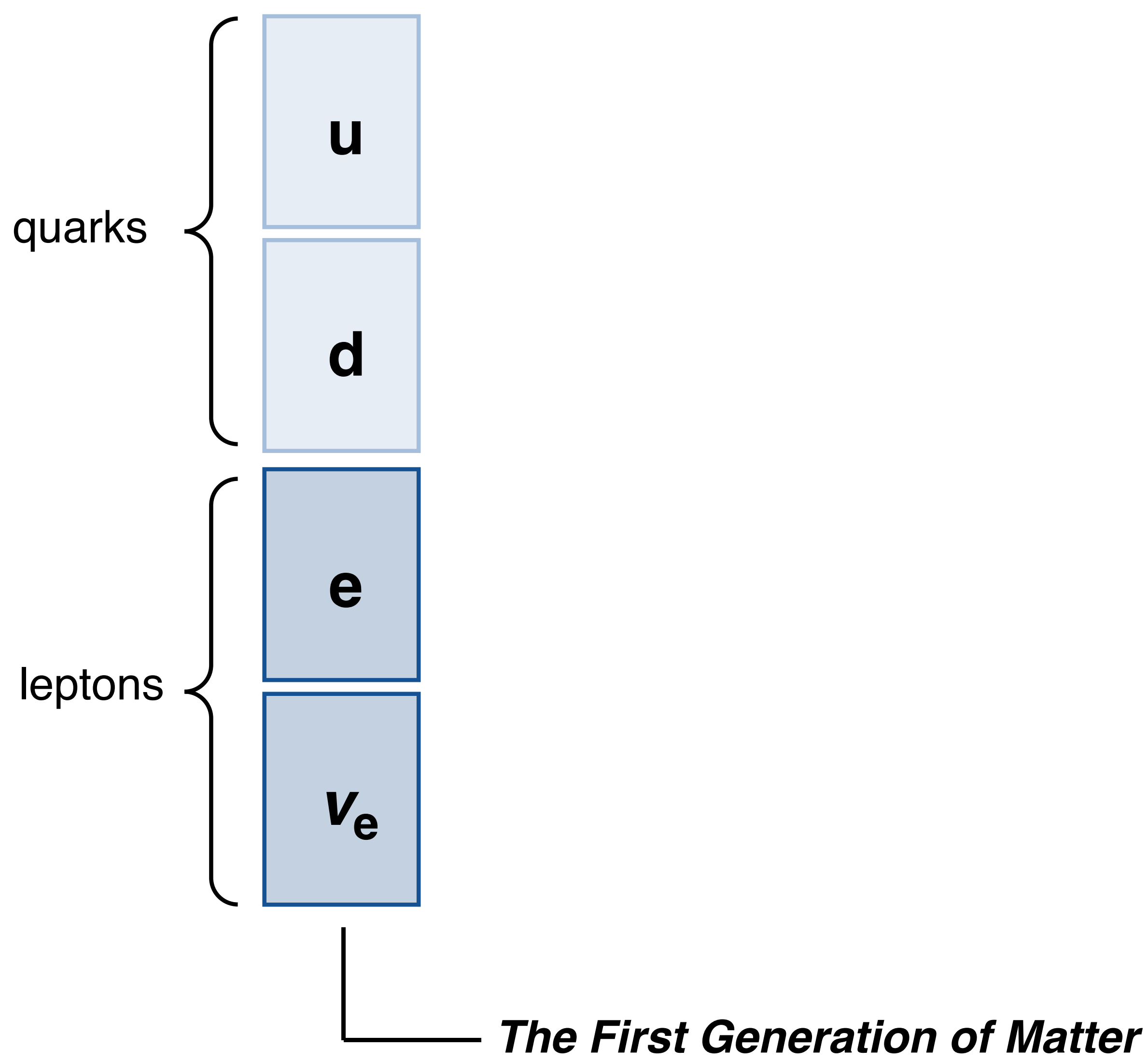
Quark: An elementary particle that experiences all four fundamental interactions

- **Up quark**: An elementary particle with charge $+^{2}/_{3}$ and spin $^{1}/_{2}$
- **Down quark**: An elementary particle with charge $-^{1}/_{3}$ and spin $^{1}/_{2}$

Quarks are the origin of proton and neutron charge and spin

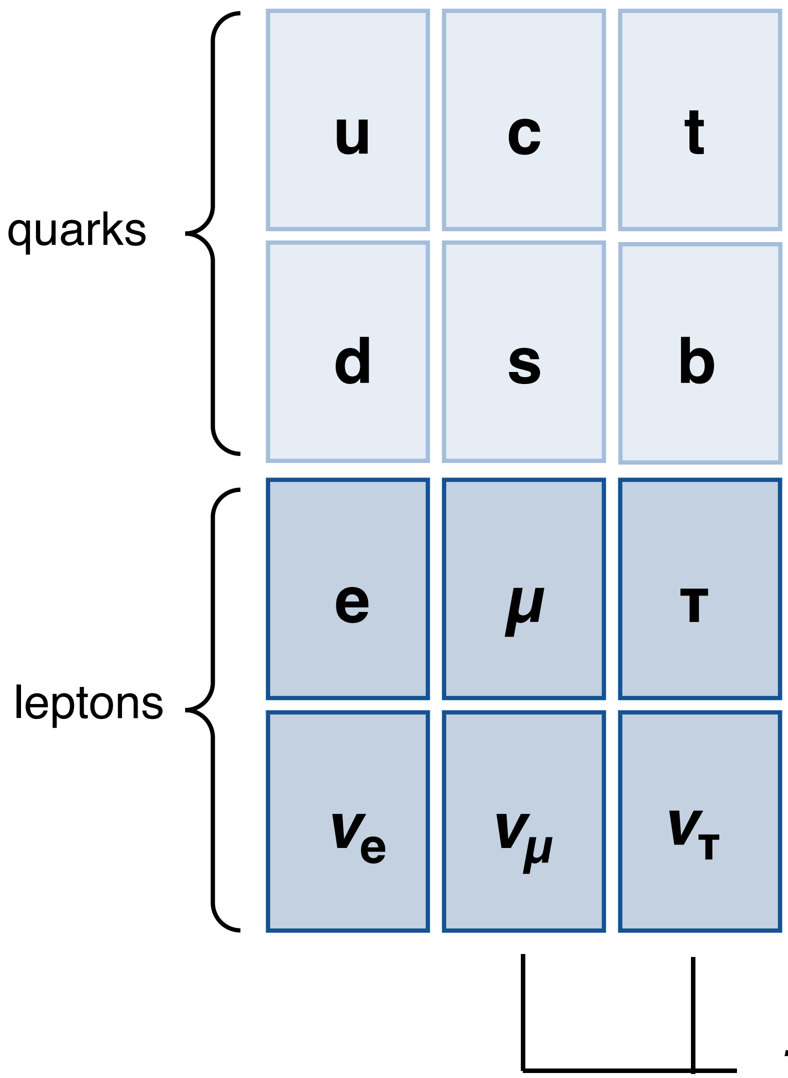
The Standard Model - An Overview

Elementary Particles



The Standard Model - An Overview

Elementary Particles



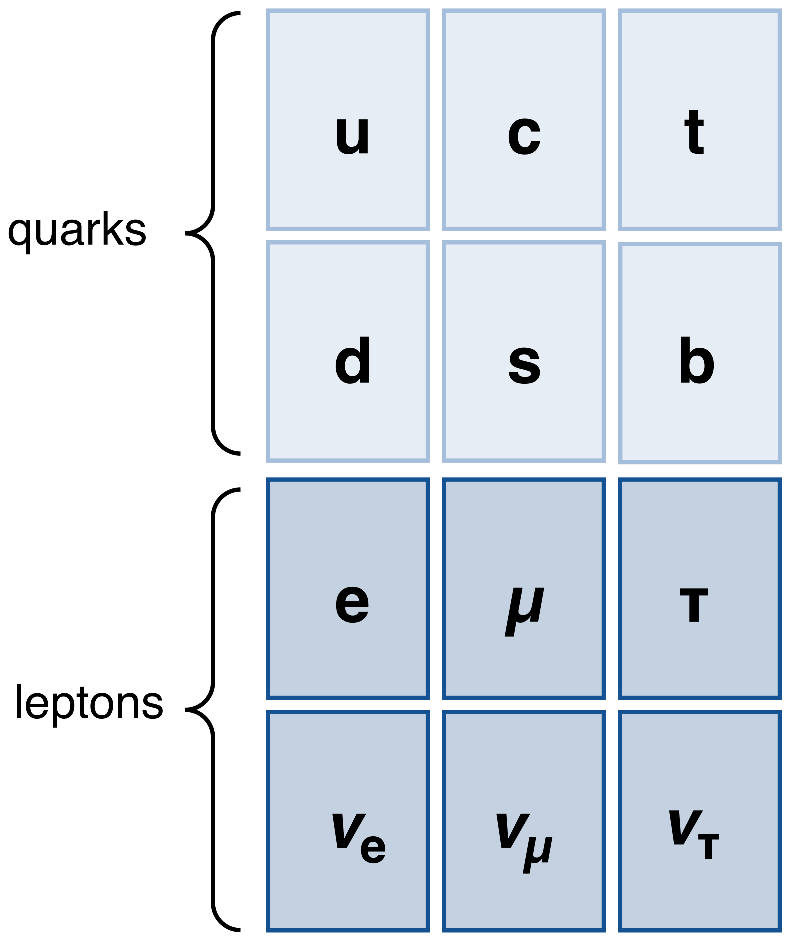
The Second and Third Generations of Matter

Heavier, substantially less stable “cousins” of first generation matter. Only detected in cosmic rays or LHC collisions

Confusing to physicist as to why these exist

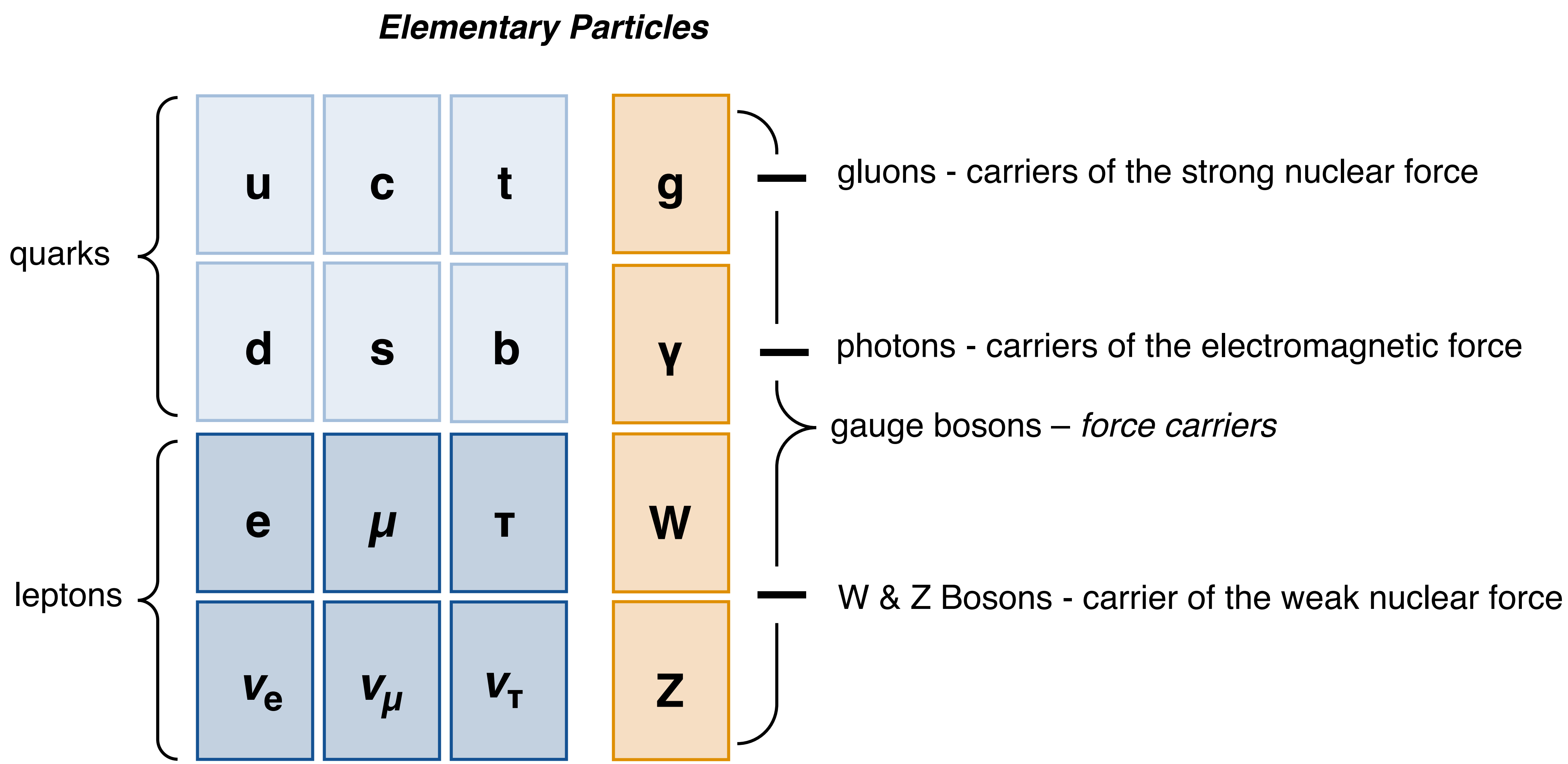
The Standard Model - An Overview

Elementary Particles



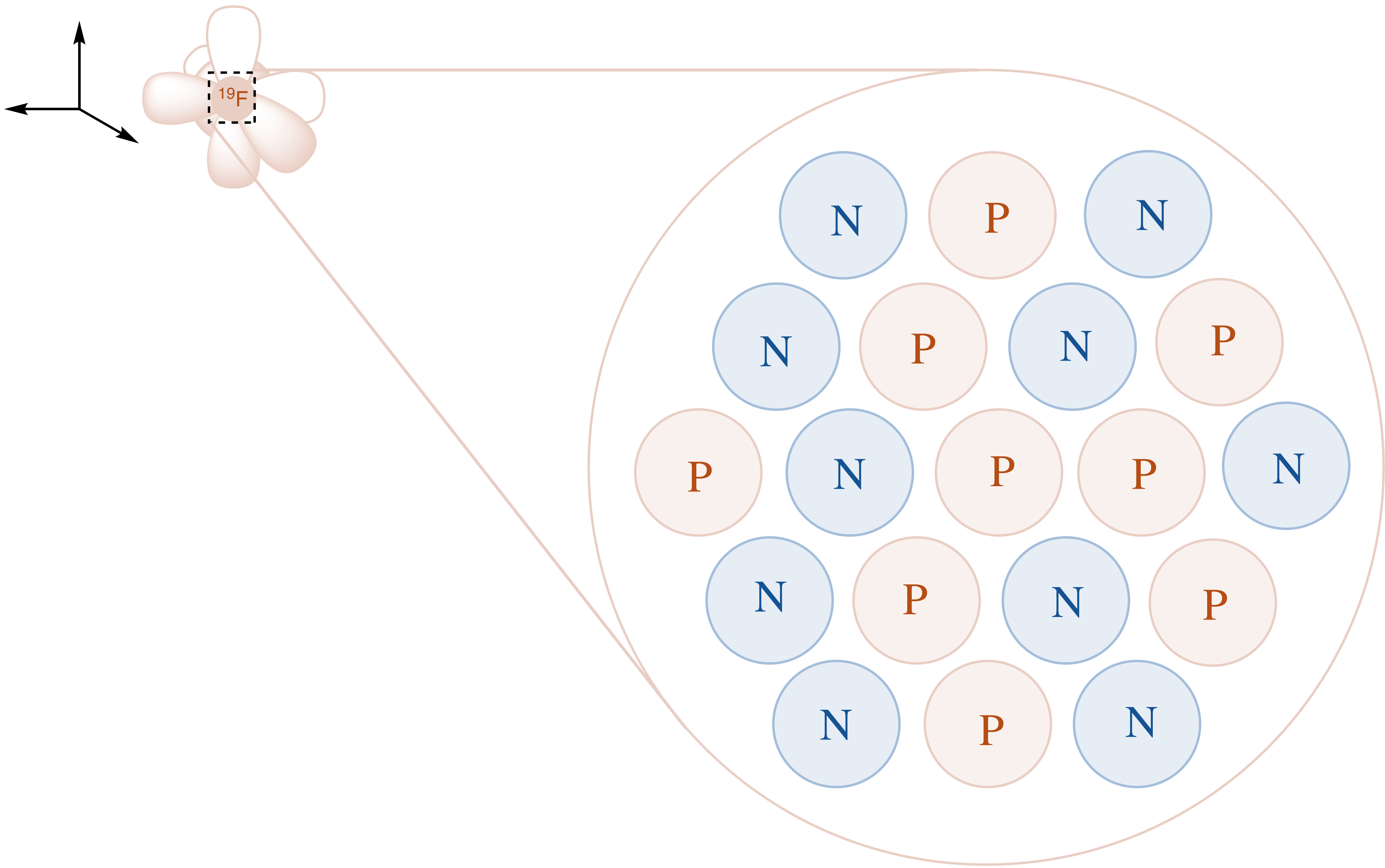
These "matter particles" or fermions are what the universe is made of, but do not explain how or why matter interacts the way it does

The Standard Model - An Overview



Particle physics still cannot accurately account for gravitational effects

Implications of the Standard Model



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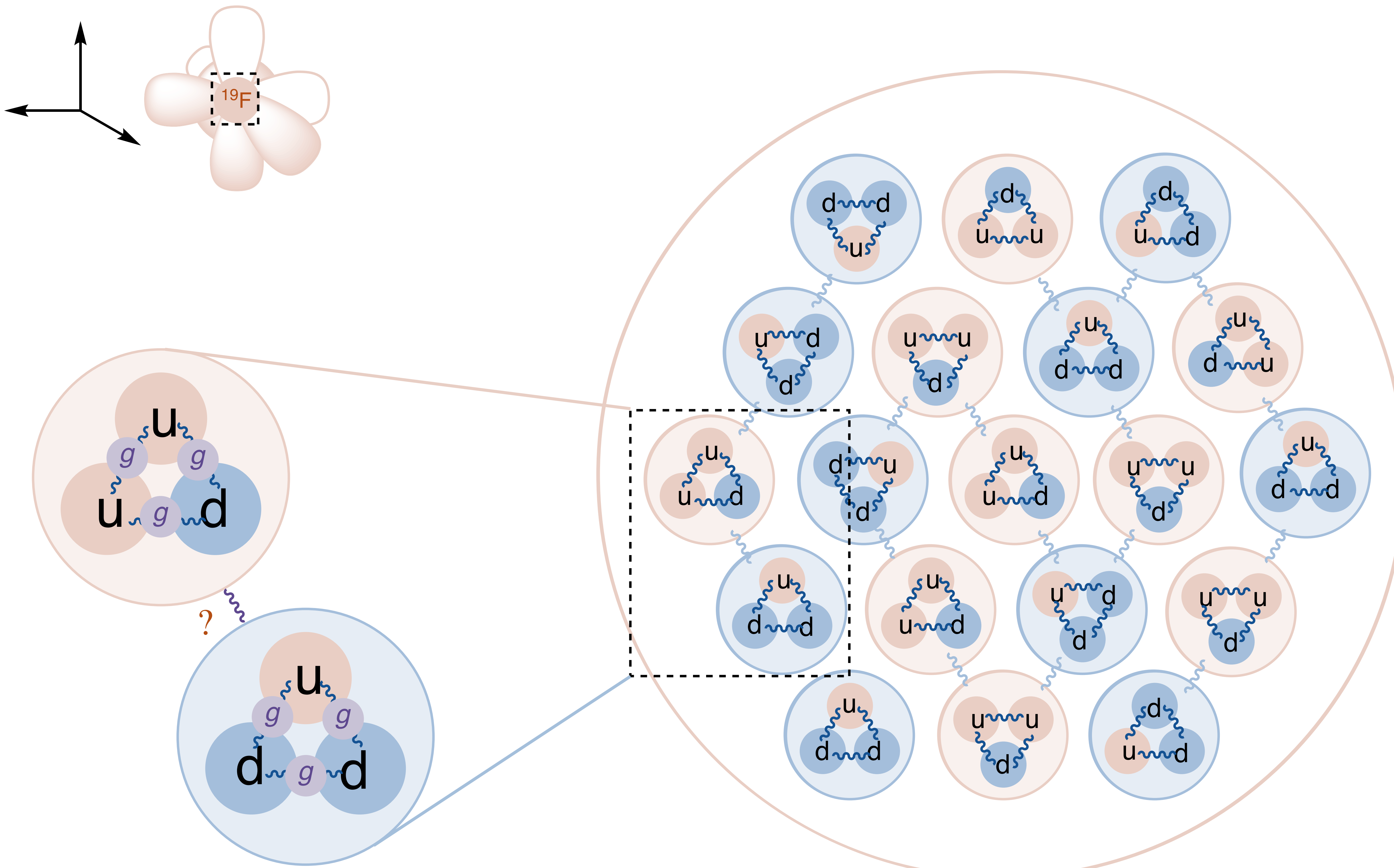
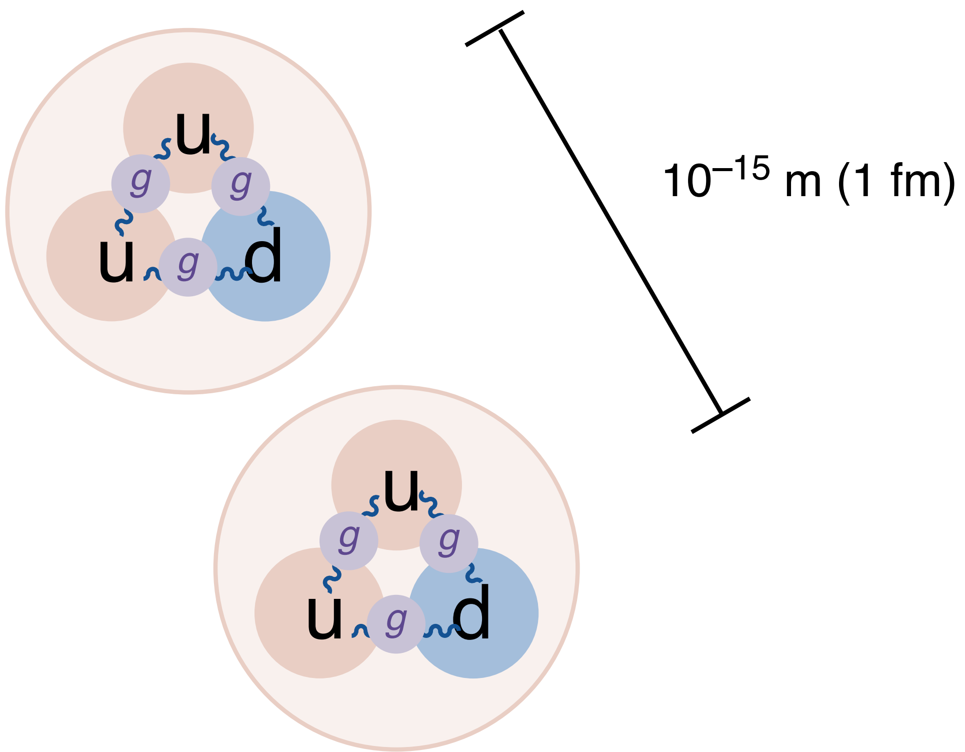


gluon exchange between quarks
“the strong interaction”

The Strong Force and the Residual Strong Force

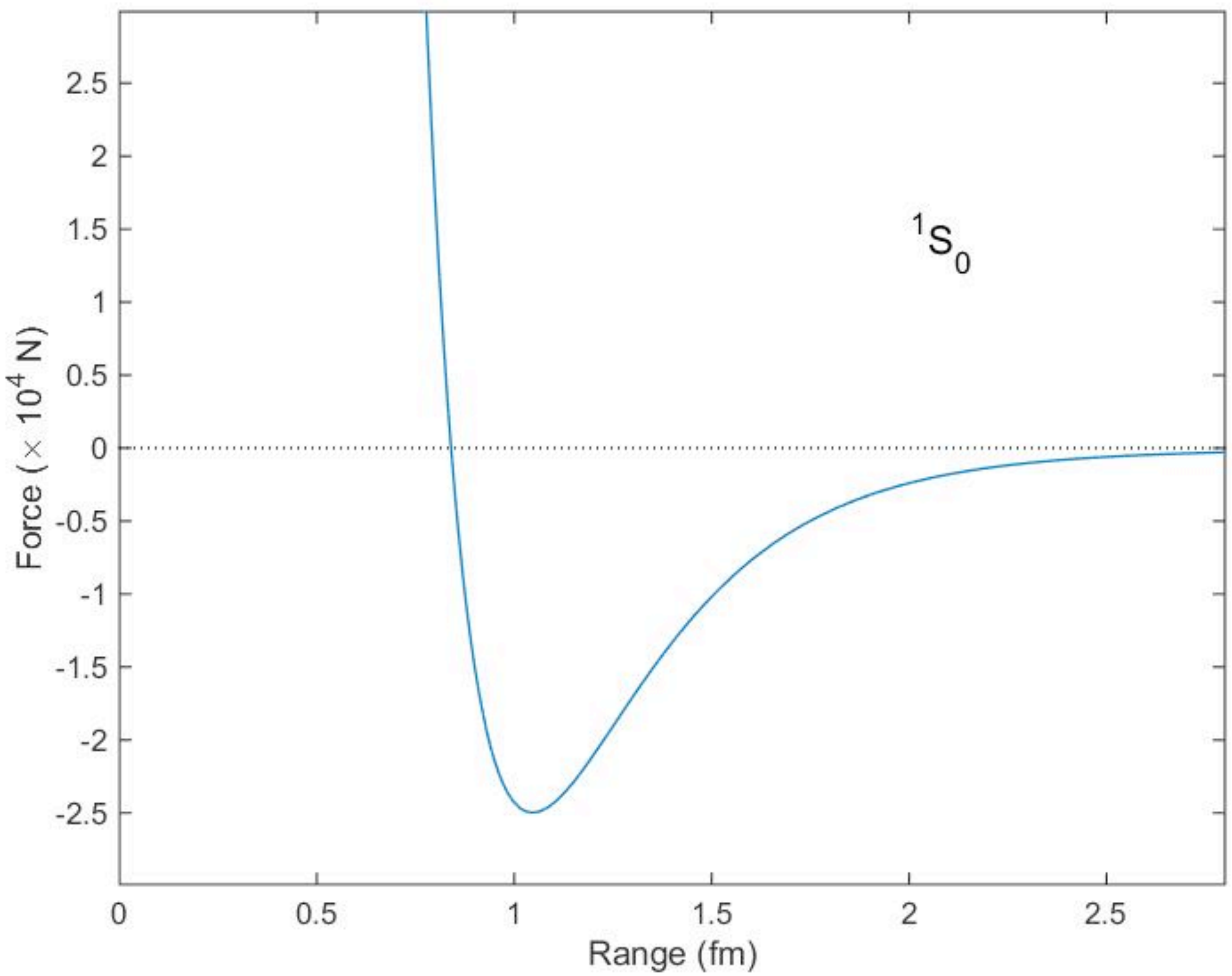


$$F(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2}$$

230 Newtons

How does nature overcome this insane barrier? The Residual Nuclear Force

The Strong Force and the Residual Strong Force

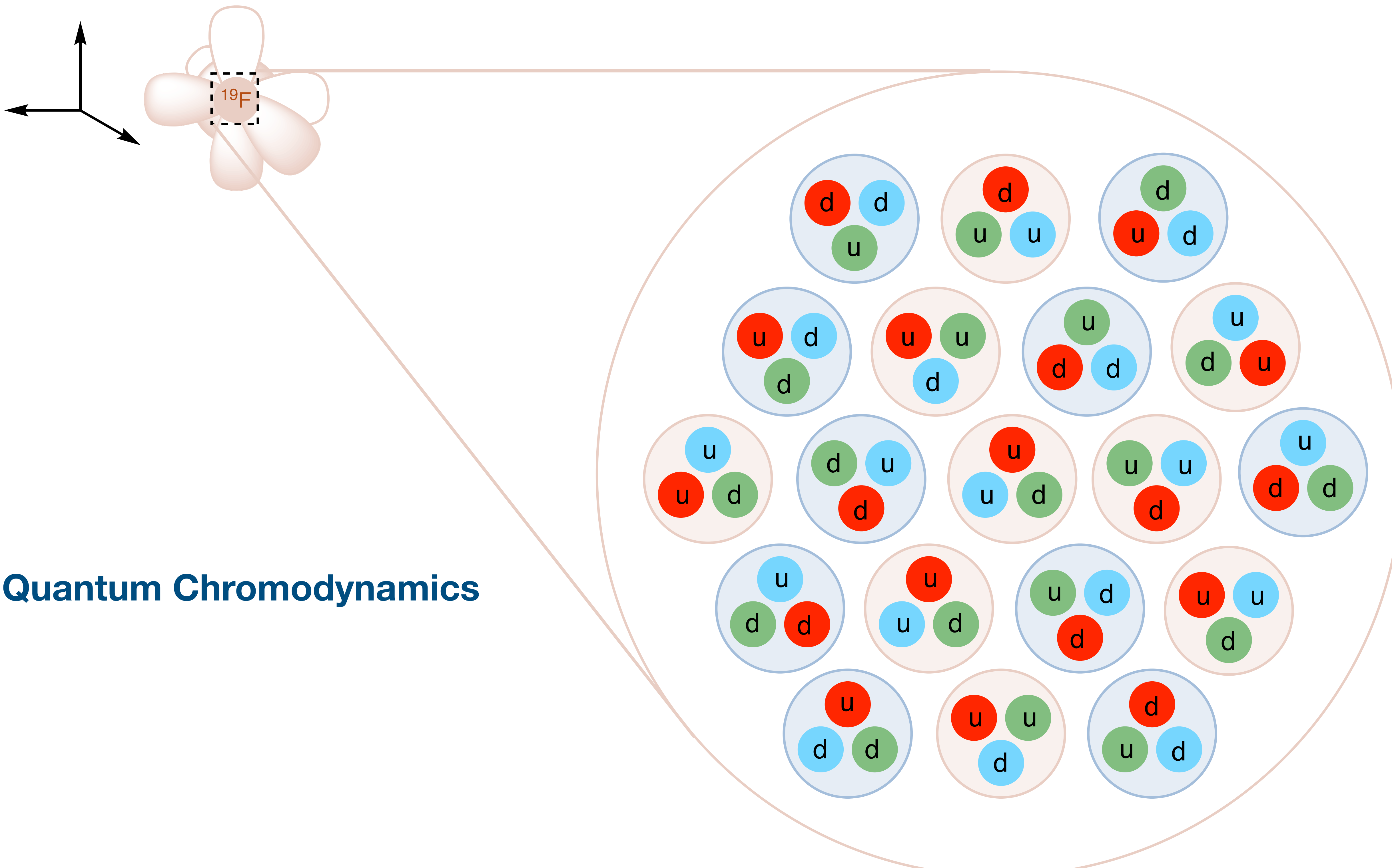


25000 Newtons

Can gluons exchange between quarks confined within different Baryons?

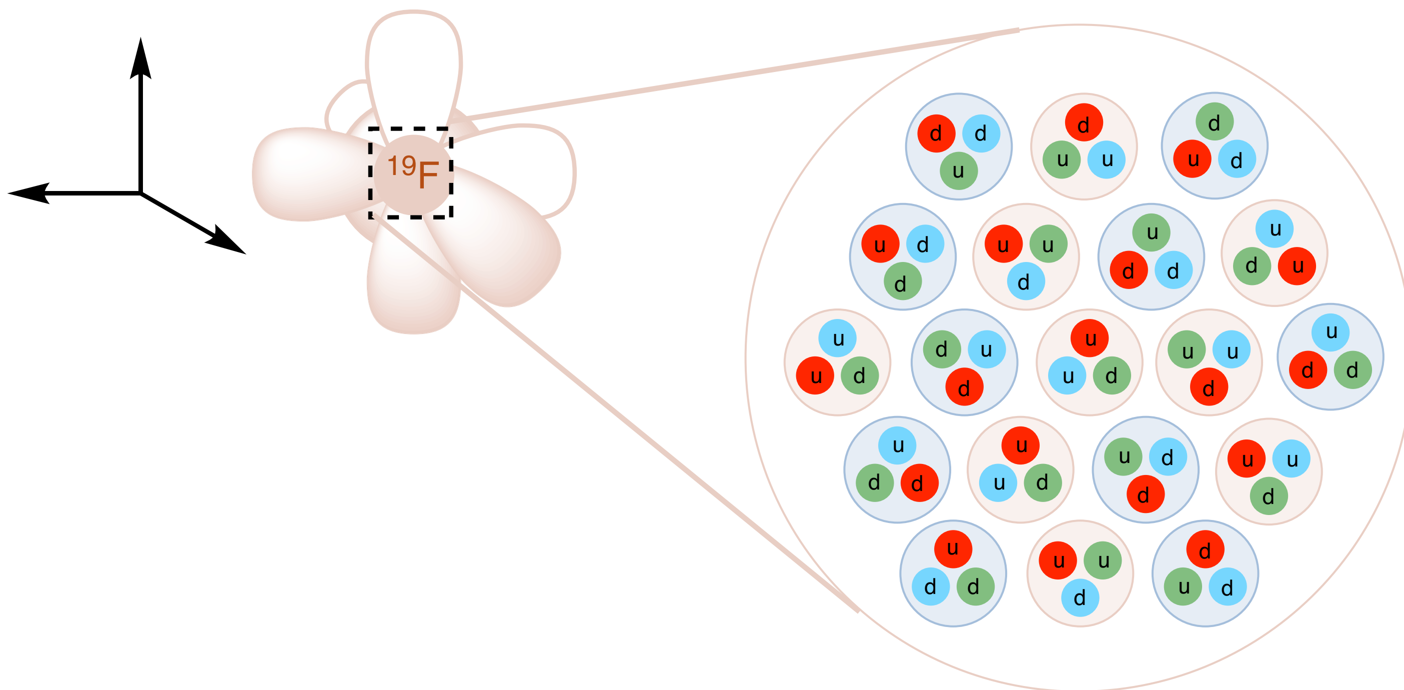
Reid, R. V. *Ann Phys-New York* **1968**, *50*, 411

A (Very) Brief Intro to QCD



Quantum Chromodynamics

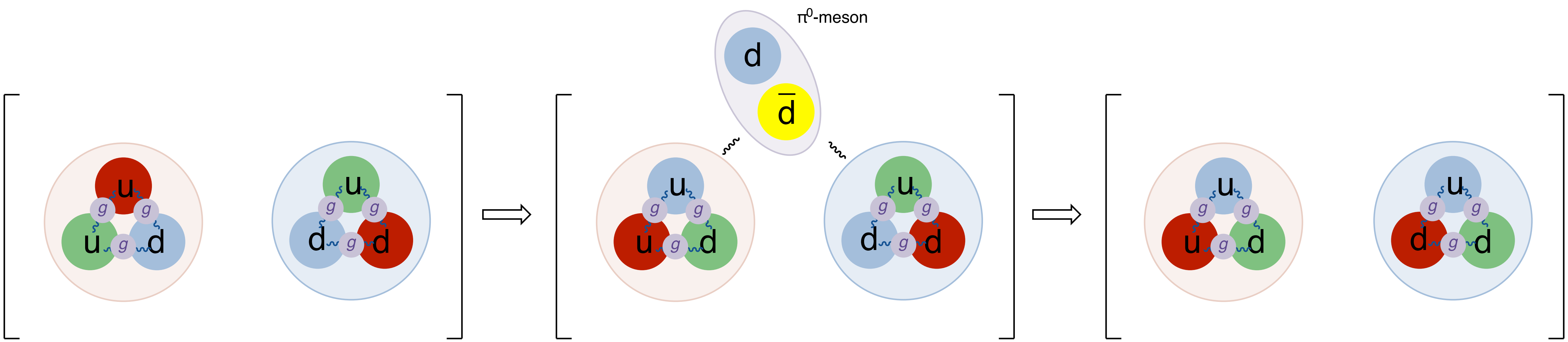
A (Very) Brief Intro to QCD



Three "colors" of strong force "charges;" each attracted to the other two by exchange of gluons

The force required to separate two quarks of a different color grows proportionally to the distance between them

Eventually, enough energy is put in to create a new quark pair, separate from the hadron



virtual meson

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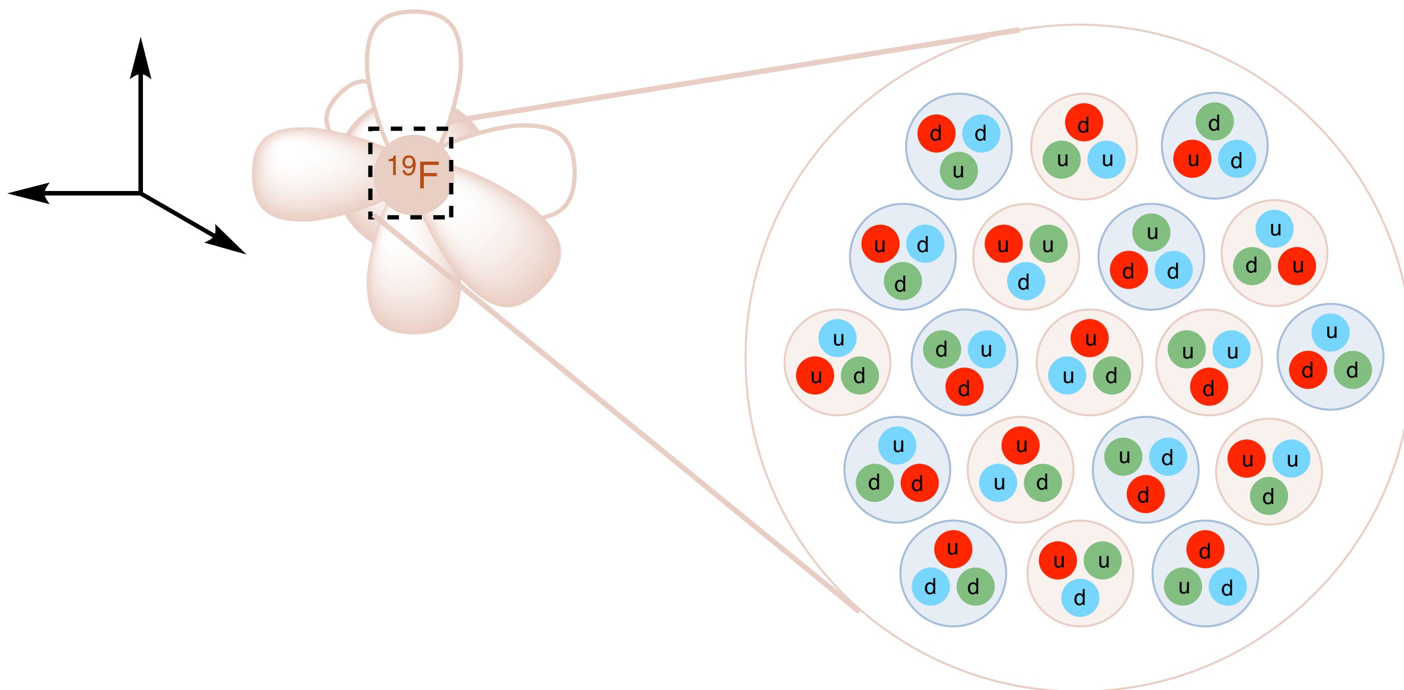

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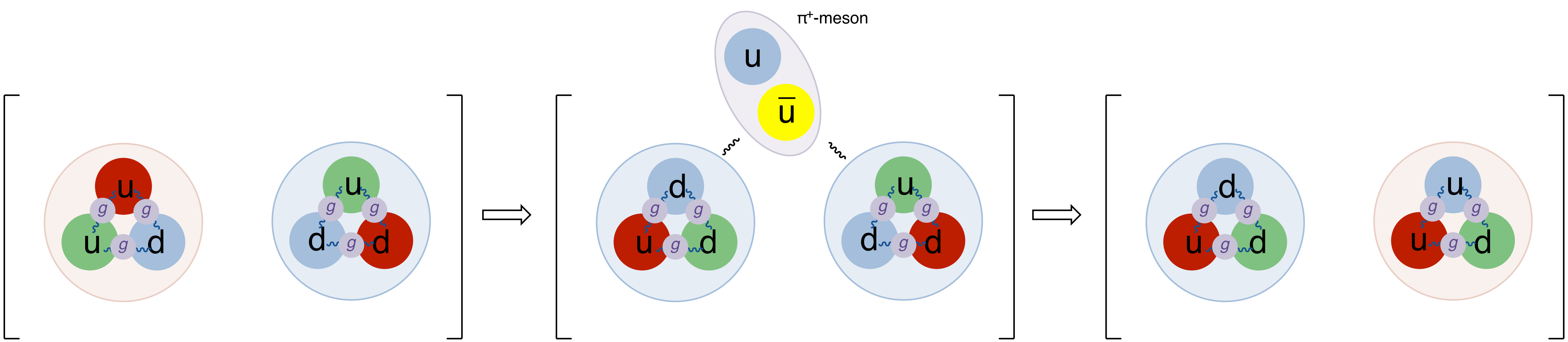


virtual meson

The Nuclear Shell Model by Analogy to the Atomic Shell Model

• ***A brief review of the atomic shell model:***

Four quantum numbers define an electron in an atom

n – principle quantum number, the energy level of the electron. Integer value from 1 to infinity

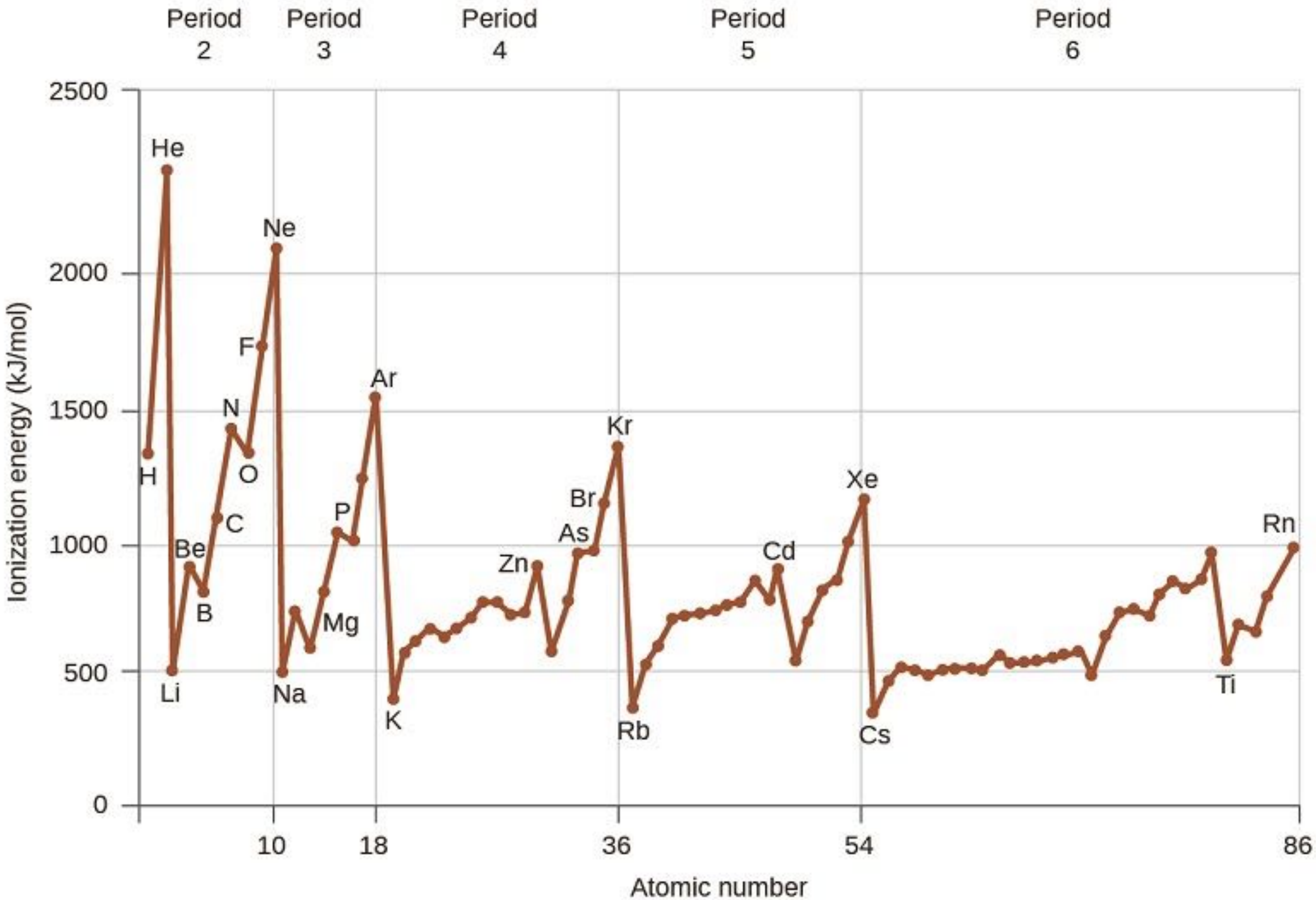
l – angular momentum quantum number, ranges from 0 to n–1. 0 = s, 1 = p, 2 = d, 3 = f, etc.

m_l – magnetic quantum number, ranges from $-l$ to l.

m_s – spin quantum number, ranges from –s to s (±1/2)

for n = 1: $l = 0$ $m_l = 0$ $m_s = {}^1/_2$ or $-{}^1/_2$	**for n = 2**: $l = 0$ or $+1$ $m_l = -1, 0,$ or $+1$ (for m≠0) $m_s = {}^1/_2$ or $-{}^1/_2$	**for n = 3**: $l = 0, +1, +2$ $m_l = -2, -1, 0, +1, +2$ (for m=2) $m_s = {}^1/_2$ or $-{}^1/_2$
2	**2 + 6**	**2 + 6 + 10**
2 = He	**10 = Ne** **18 = Ar**	**36 = Kr**

The Nuclear Shell Model by Analogy to the Atomic Shell Model



The Nuclear Shell Model

- ***Application to the Nuclear Shell Model***

Four quantum numbers define a Nucleon, with Neutrons and Protons treated independently

n – principle quantum number, the energy level of the electron. Integer value from 1 to infinity

l – angular momentum quantum number, **not restricted by n**

m_l – magnetic quantum number, ranges from –l to l.

m_s – spin quantum number, ranges from –s to s (±1/2)

This treatment affords filled shell numbers of ***2, 8, 20, 28, 50, 82, 126***

Magic nuclei: Nuclei with an atomic number or neutron number that is "magic" (a filled shell) (^{58}**Ni***)*

Doubly magic nuclei: Nuclei with both an atomic number and neutron number that is "magic" (^{48}**Ni***)*

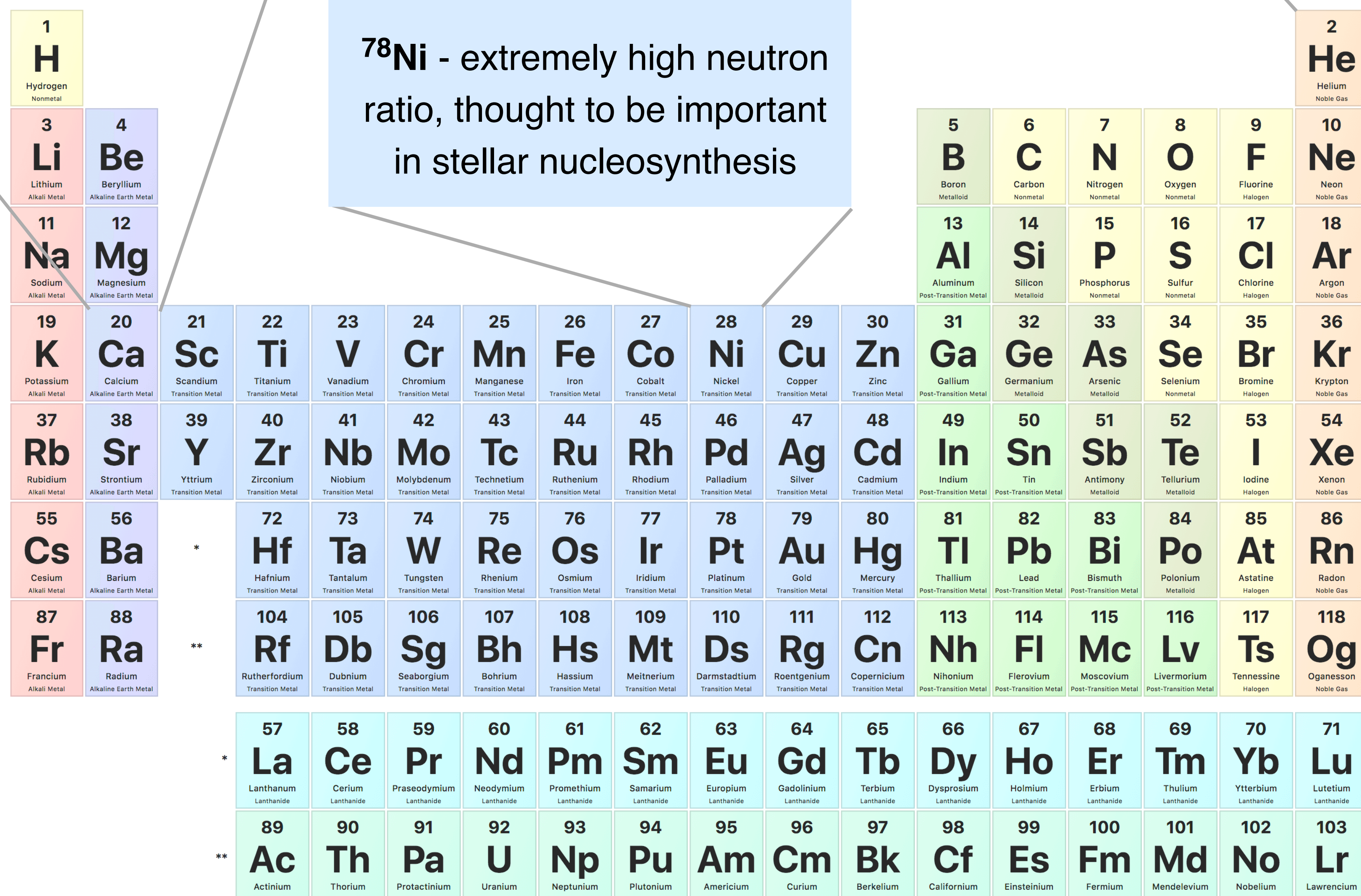
The Nuclear Shell Model

^{40}**Ca** - heaviest stable nuclide where N = Z

^{48}**Ni** - the most proton rich nuclide beyond ^{3}He (28 + 20)

^{78}**Ni** - extremely high neutron ratio, thought to be important in stellar nucleosynthesis

^{10}**He** is doubly-magic (10^3 longer lived than ^{5}**He**)



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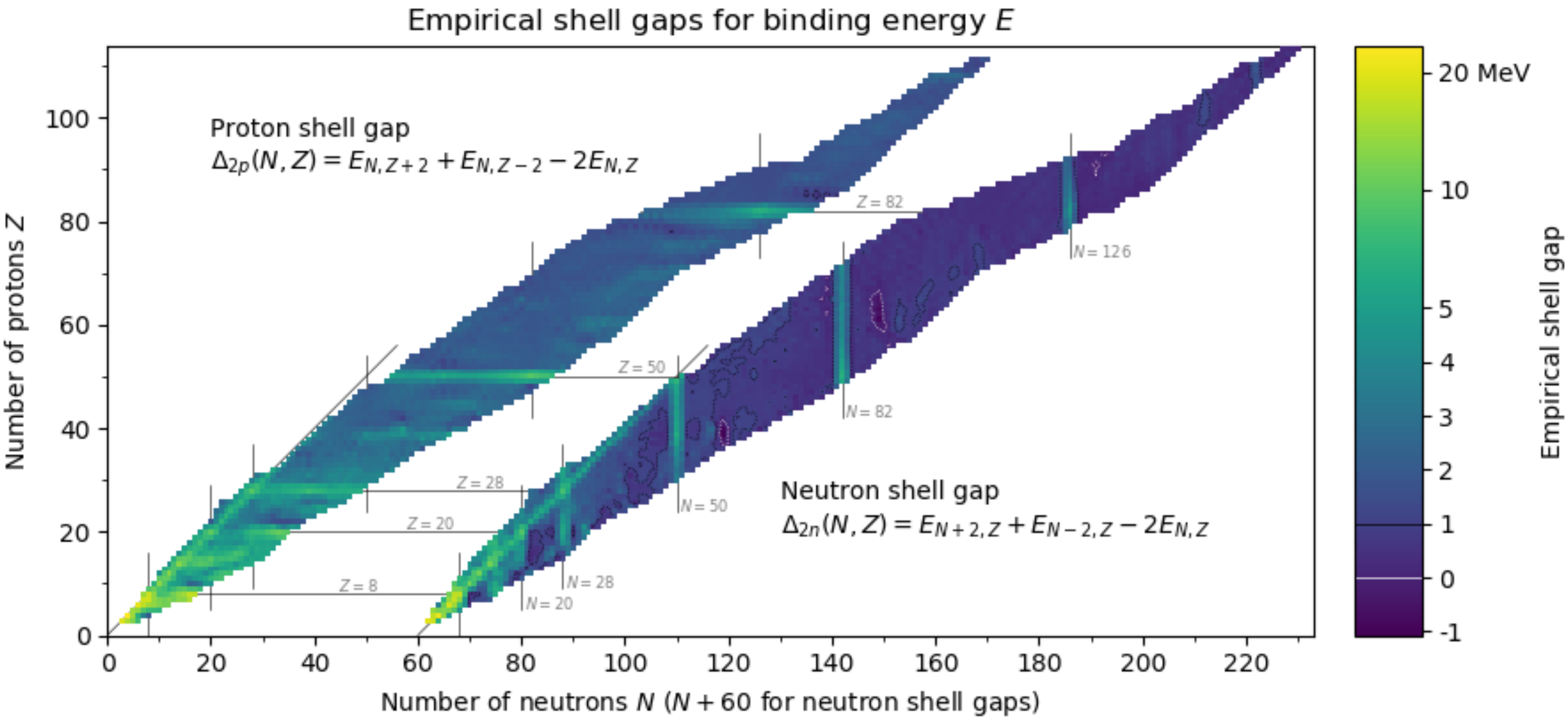
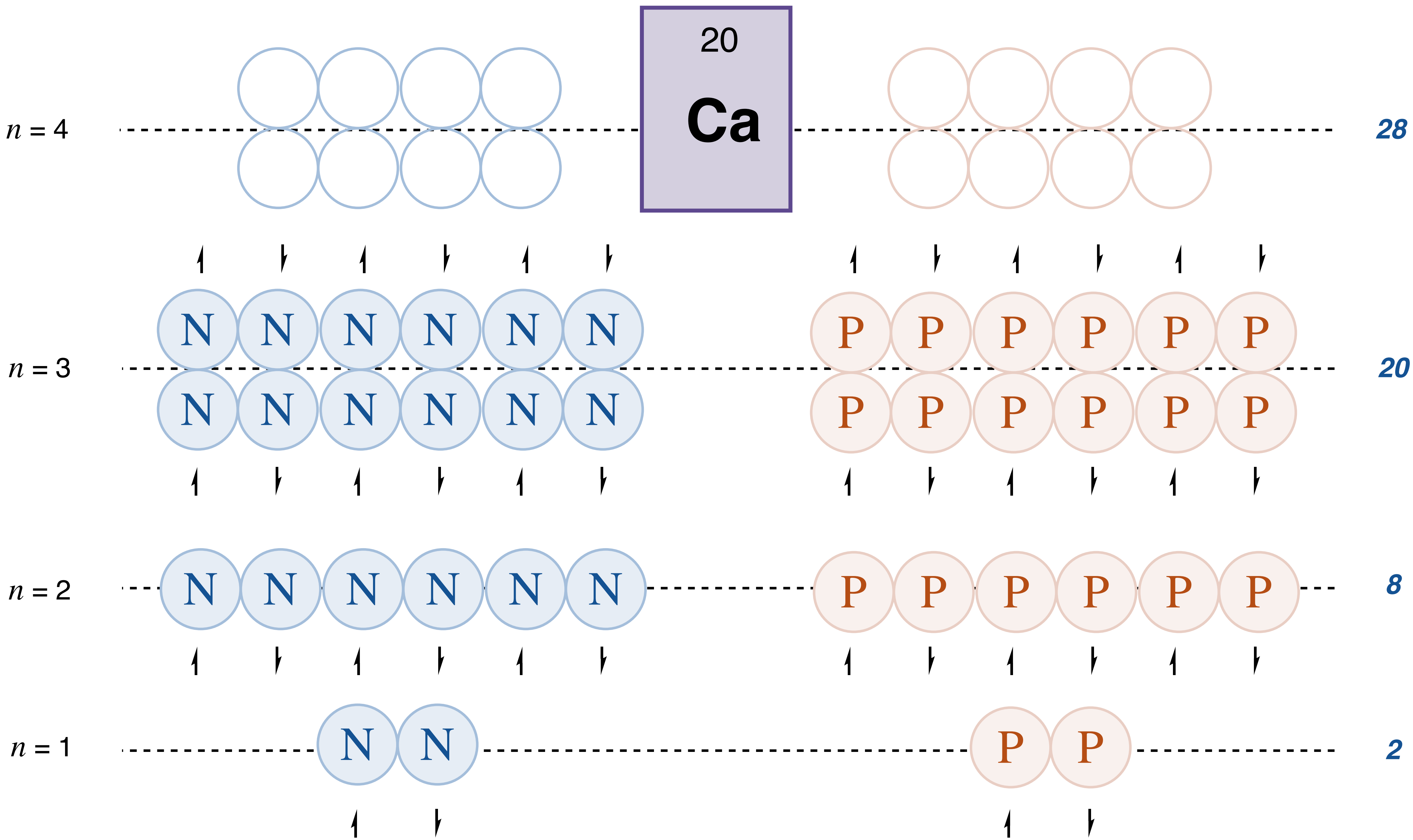


Magic numbers are calculated only for ***spherical nuclei***

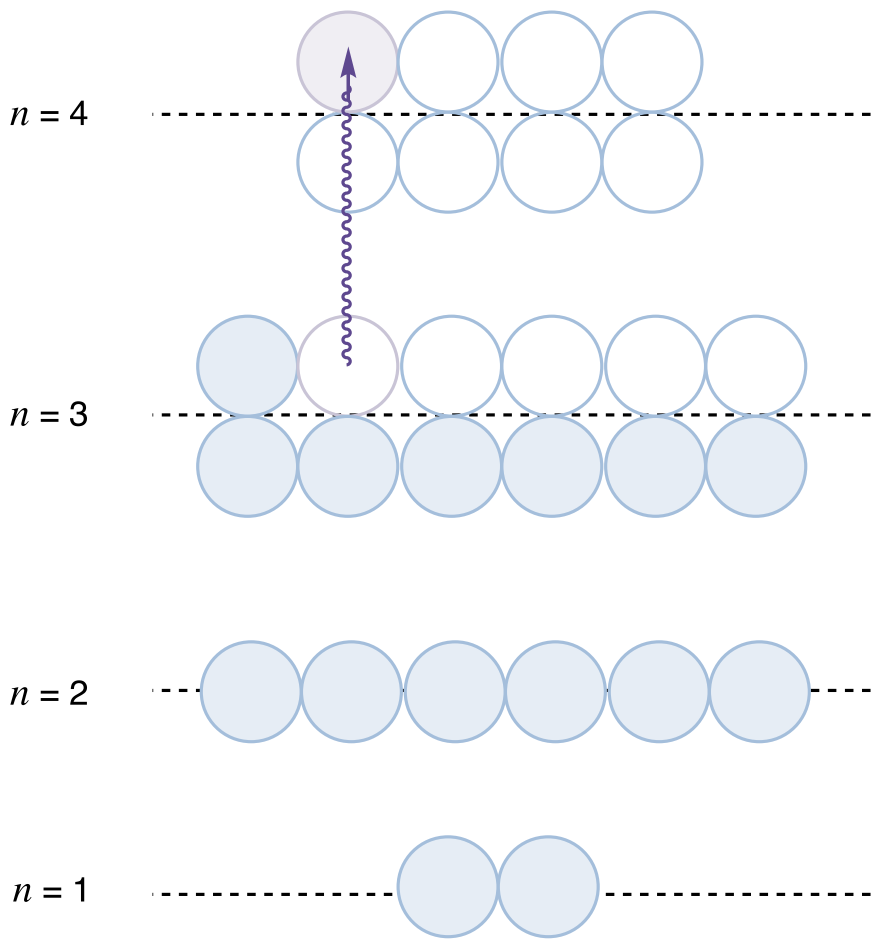
Magic numbers (or semi-magic numbers) can be empirically derived from these tables

The Nuclear Shell Model

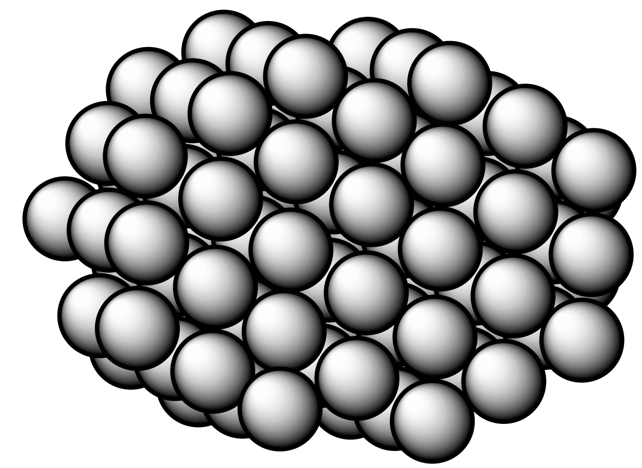


Nuclear Excited States

Nuclear Transition (Shell Theory)



Vibrational and Rotational Excitation in Deformed Nuclei (Collective Theory)



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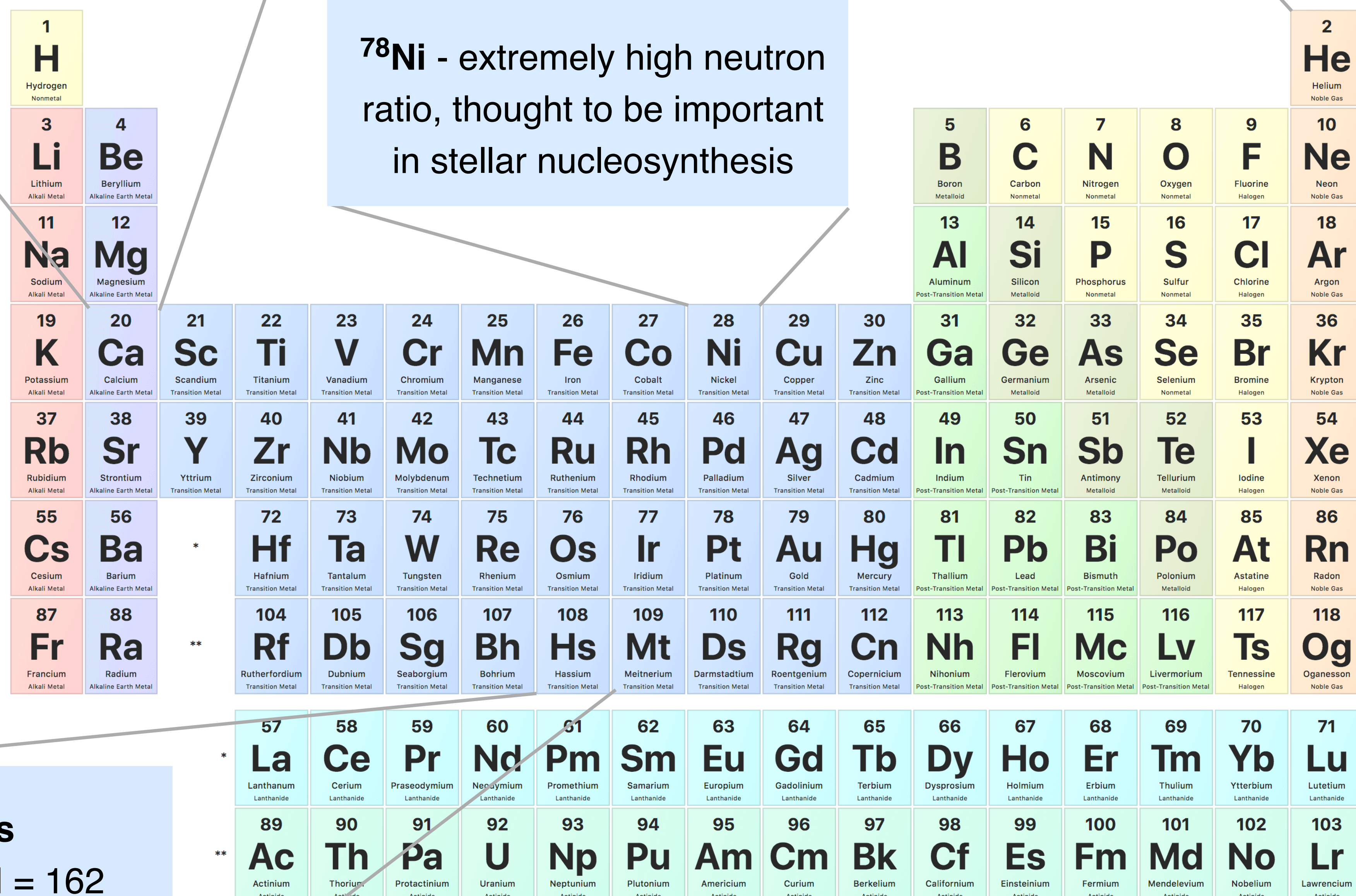


^{270}**Hs**

Z = 108, N = 162

doubly magic for deformed nuclei

Nuclear Isomers

Nuclear excited states typically decay within 10^{-12} s

Nuclear excited states that are longer lived than 1 ns (10^{-9} s) are considered nuclear isomers

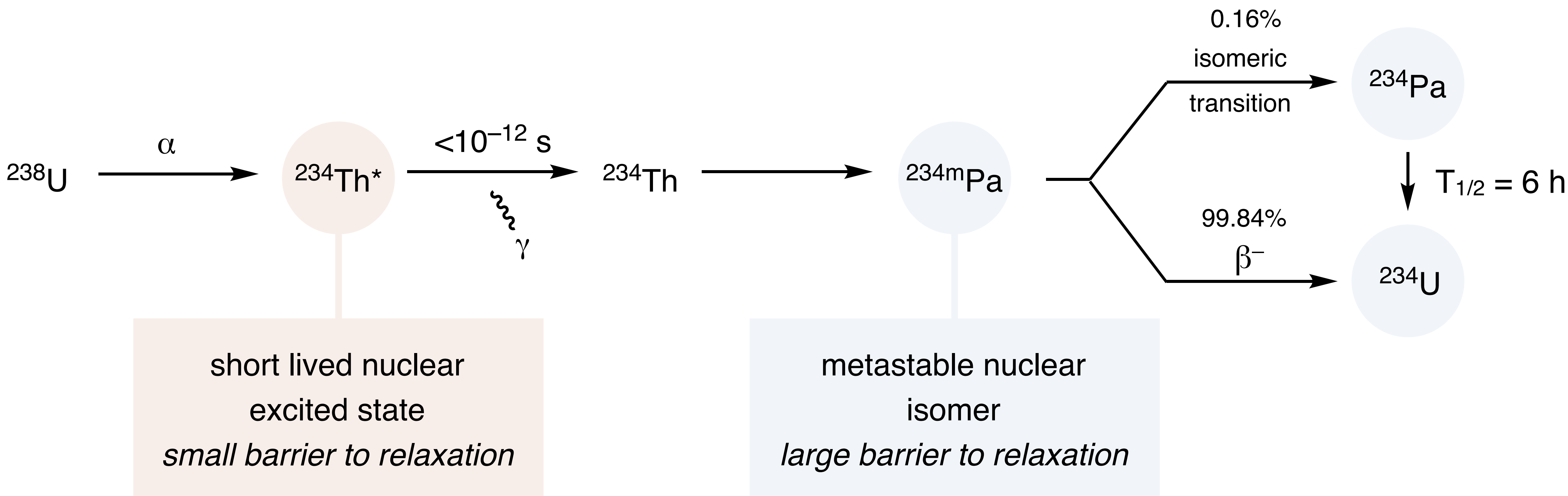
Metastable isomers are traditionally nuclear reaction products that are formed in an excited state (e.g. via the conversion of a neutron to a proton in an unusual spin state)

$$^{234}\mathrm{Th} \xrightarrow{\beta^-} {}^{234m}\mathrm{Pa}$$

protactinium was discovered as it's metastable state! ($T_{1/2}$ = 1.17 minutes)

Metastable Nuclear Isomers

Typical decay chain: A case study



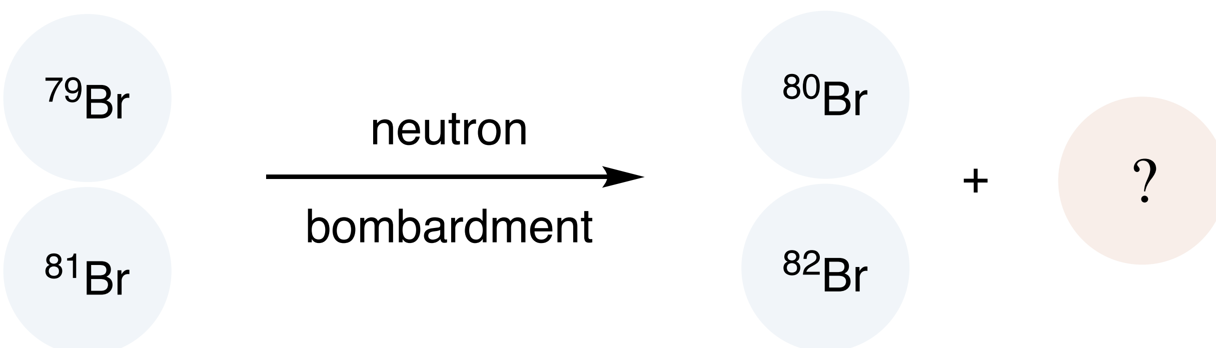
Isomeric transition: Decay of nuclear isomer/excited state to a lower energy state

gamma emission	**internal conversion**
analogous to electronic excited state decay via photon emission	*an electron couples to the excited nucleus, and relaxation of the nucleus ejects the electron (note: this is different from β decay)*

Notable Nuclear Isomers: ^{80m}Br

1934: Kurchatov and coworkers publish on the neutron bombardment of a commercial Br_2 sample.

Three distinct beta-emitting isotopes are detected



Rusinov, L. I. *Usp. Fiz. Nauk.* **1961**, *73*, 615

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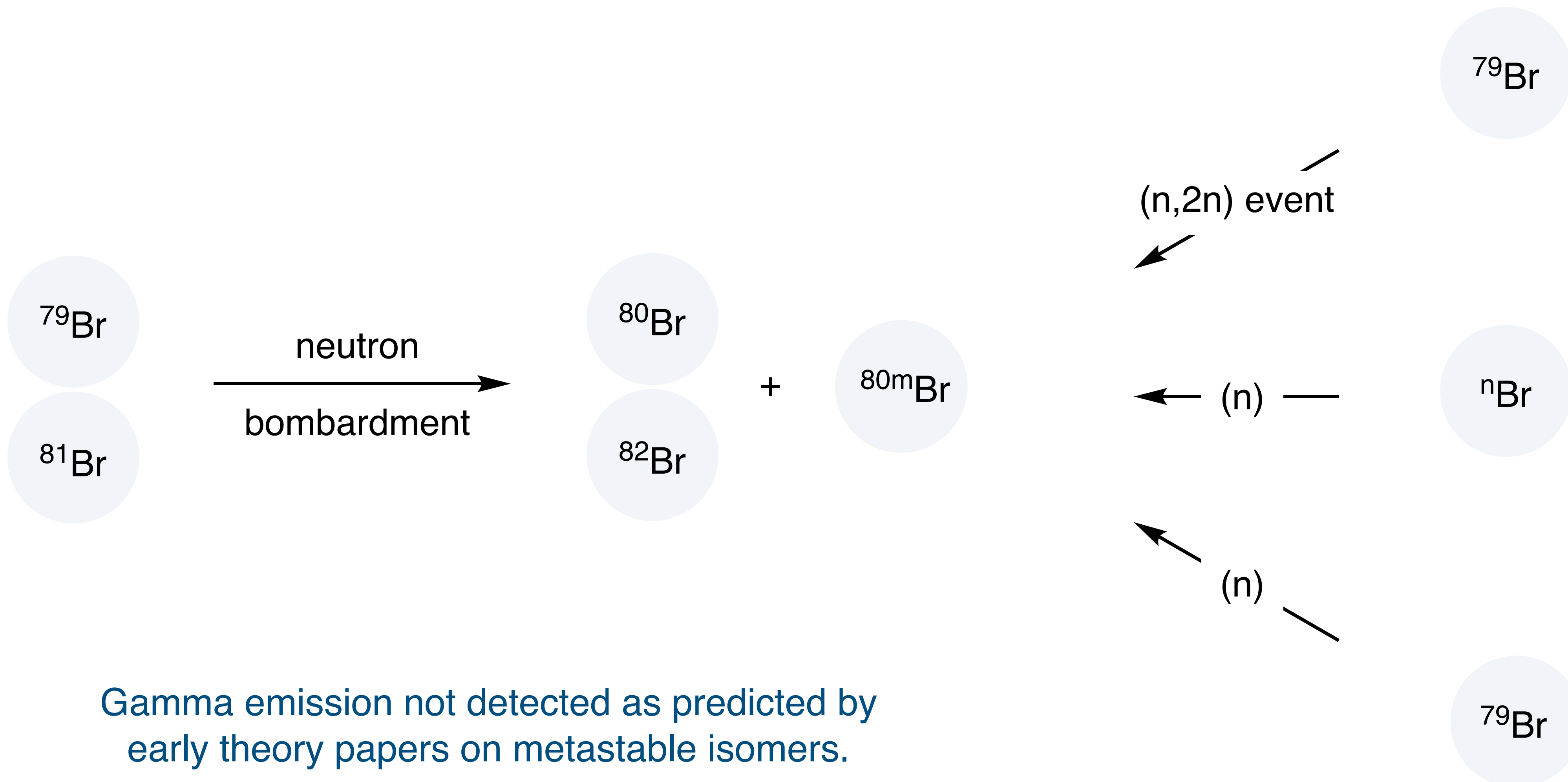


Gamma emission not detected as predicted by early theory papers on metastable isomers.

Internal conversion mistaken for β decay

Rusinov, L. I. *Usp. Fiz. Nauk.* **1961**, *73*, 615

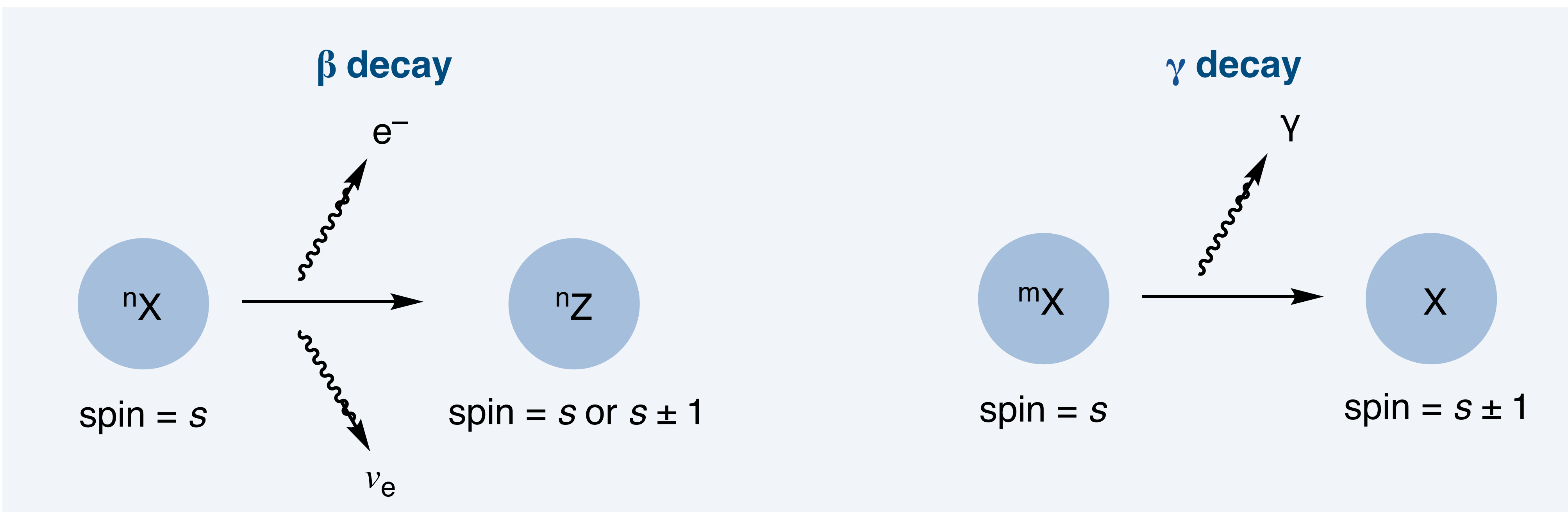
Notable Nuclear Isomers: ^{180m1}Ta

^{180}Ta is a spin = 1 nucleus with an odd number of both protons and neutrons (odd/odd nucleus)

$T_{1/2}$ = 8.1 h: electron capture to ^{180}Hf or β^- to ^{180}W

^{180m1}Ta: The rarest primordial nuclide in the universe - observationally stable

$T_{1/2} > 10^{16}$ years



Each additional (forbidden) unit of angular momentum slows the relaxation process by 10^5

Lehnert, B.; Hult, M.; Lutter, G.; Zuber, K. *Phys Rev C* **2017**, *95*, 044306

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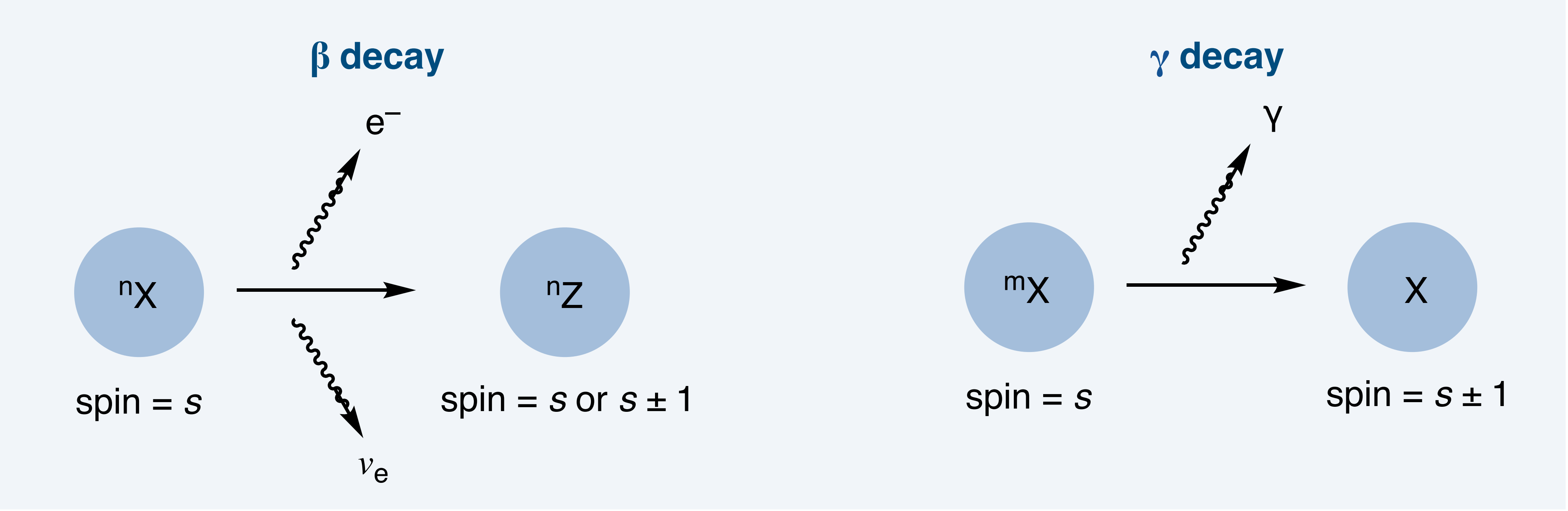


What imparts this exceptional stability against all decay pathways of ^{180m1}Ta?

Nuclear spin = 9! Any decay pathway is "exceptionally forbidden"
Rate decrease of 10^{5^7}

Lehnert, B.; Hult, M.; Lutter, G.; Zuber, K. *Phys Rev C* **2017**, *95*, 044306

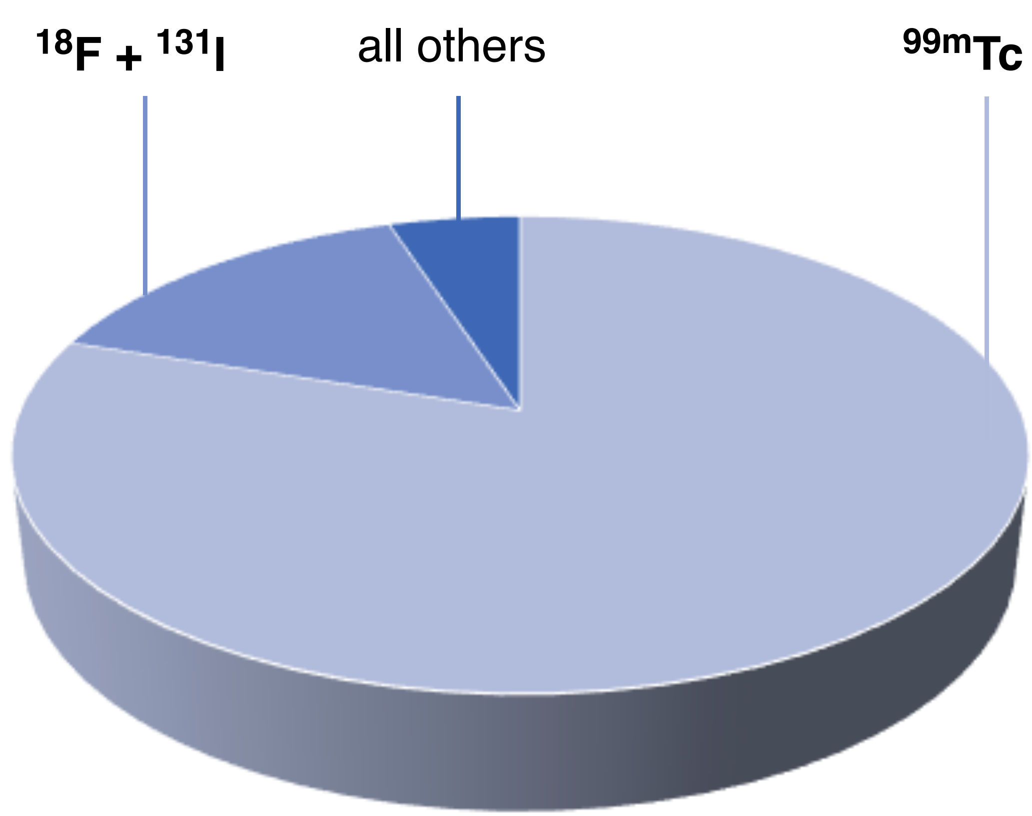
Notable Nuclear Isomers: ^{99m}Tc

43
Tc
technetium

exceedingly rare as a naturally occuring element due to short half lives of all naturally occuring isotopes (<4.2 My)

all technetium used for radiochemical applications is produced synthetically

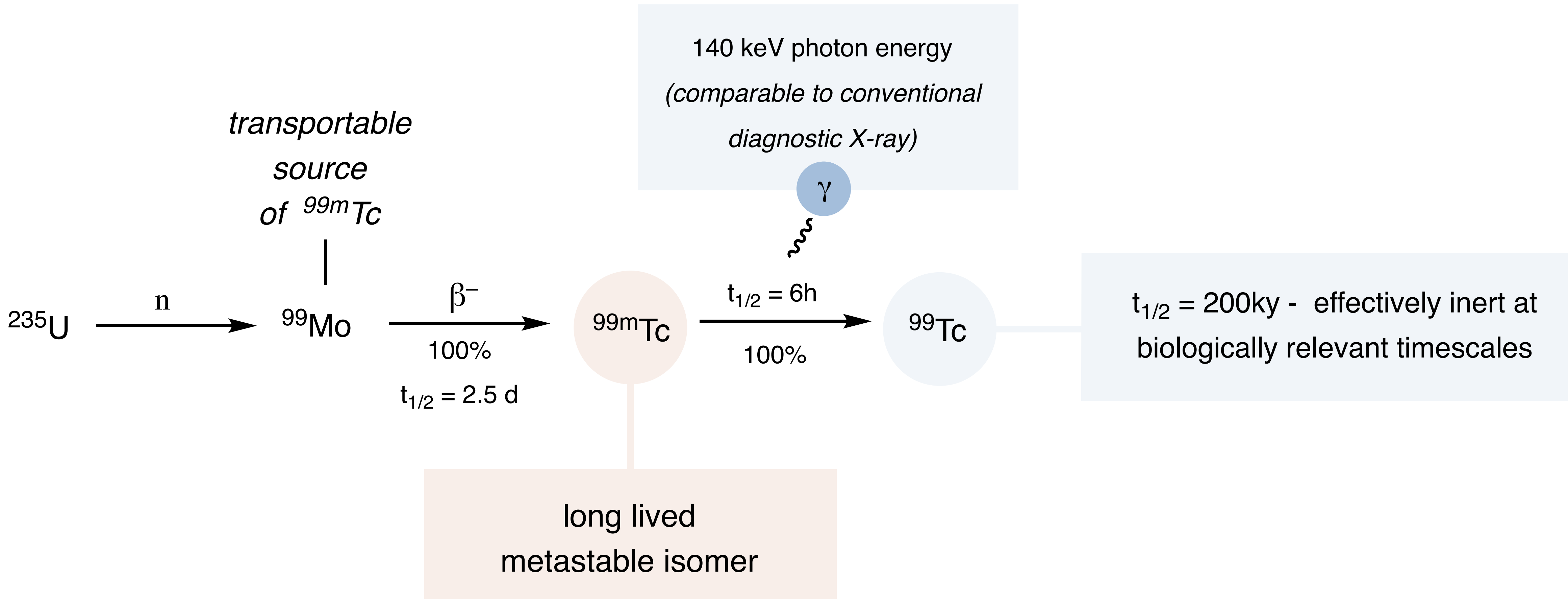
The metastable isomer ^{99m}Tc has extensive applications as a medical radioisotope



Askbar, M. U.; Ahmad, M. R.; Shaheen, A.; Mushtaq, S. *J. Radioanal. Nucl. Chem.* **2016**, *310*, 477

Hjelstuen, O. K. *The Analyst* **1995**, *120*, 863

Notable Nuclear Isomers: ^{99m}Tc



clean gamma emission only - easily detectable by gamma cameras
no alpha or beta particles *in vivo*

Askbar, M. U.; Ahmad, M. R.; Shaheen, A.; Mushtaq, S. *J. Radioanal. Nucl. Chem.* **2016**, *310*, 477

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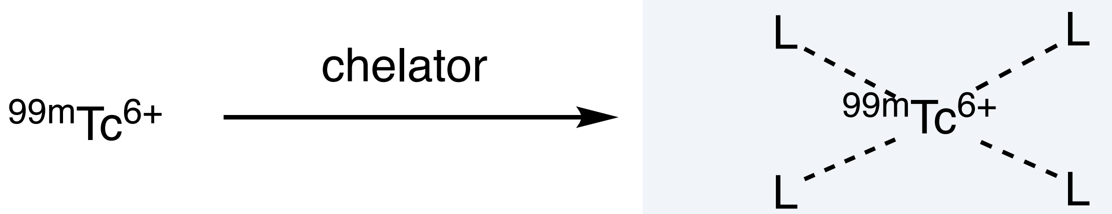
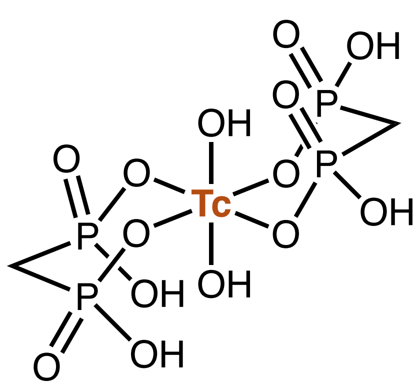
Notable Nuclear Isomers: ^{99m}Tc

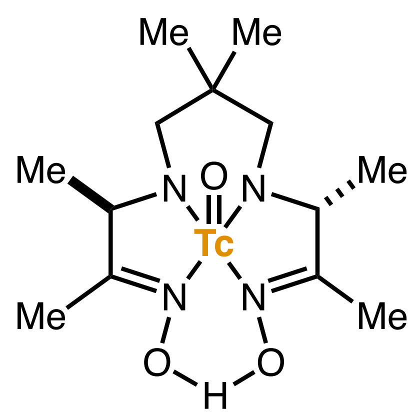


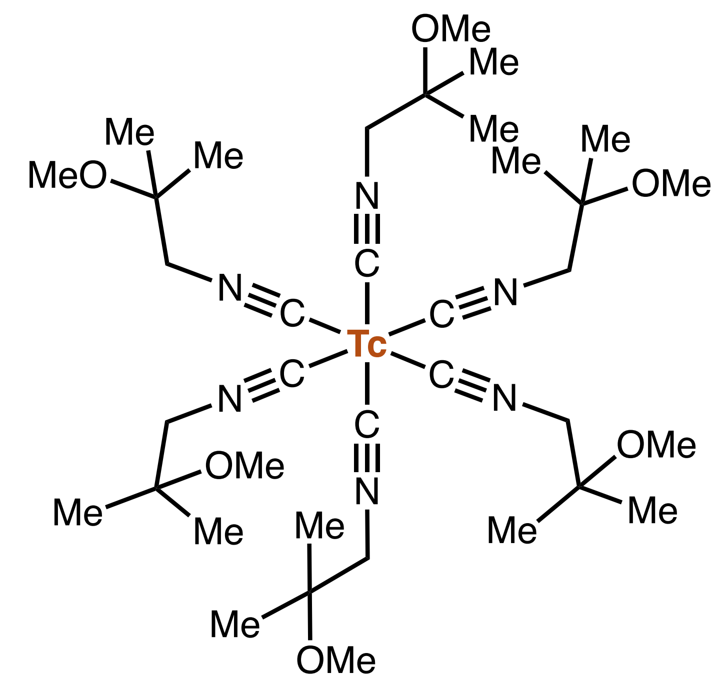
purified to >99% RCP

with commercial kits

chelator/ligand sphere is adjusted for specific applications and site specificity







^{99m}Tc(MDP)$_2$

selectively absorbed by bone cells

localizes in bone cancers

^{99m}Tc-exametazime

localizes in regions of impaired neurological activity

used in stroke diagnoses

^{99m}Tc-HMIBI

cationic complex selectively absorbed by heart cells

used in cardiovascular diagnoses

Askbar, M. U.; Ahmad, M. R.; Shaheen, A.; Mushtaq, S. *J. Radioanal. Nucl. Chem.* **2016**, *310*, 477

Hjelstuen, O. K. *The Analyst* **1995**, *120*, 863

Notable Nuclear Isomers: ^{229m}Th

LETTER

https://doi.org/10.1038/s41586-019-1533-4

Energy of the ^{229}Th nuclear clock transition

Benedict Seiferle[1]*, Lars von der Wense[1], Pavlo V. Bilous[2], Ines Amersdorffer[1], Christoph Lemell[3], Florian Libisch[3], Simon Stellmer[4], Thorsten Schumm[5], Christoph E. Düllmann[6,7,8], Adriana Pálffy[2] & Peter G. Thirolf[1]

LETTER

https://doi.org/10.1038/s41586-019-1542-3

X-ray pumping of the ^{229}Th nuclear clock isomer

Takahiko Masuda[1], Akihiro Yoshimi[1], Akira Fujieda[1], Hiroyuki Fujimoto[2], Hiromitsu Haba[3], Hideaki Hara[1], Takahiro Hiraki[1], Hiroyuki Kaino[1], Yoshitaka Kasamatsu[4], Shinji Kitao[5], Kenji Konashi[6], Yuki Miyamoto[1], Koichi Okai[1], Sho Okubo[1], Noboru Sasao[1]*, Makoto Seto[5], Thorsten Schumm[7], Yudai Shigekawa[4], Kenta Suzuki[1], Simon Stellmer[7,10], Kenji Tamasaku[8], Satoshi Uetake[1], Makoto Watanabe[6], Tsukasa Watanabe[2], Yuki Yasuda[4], Atsushi Yamaguchi[3], Yoshitaka Yoda[9], Takuya Yokokita[3], Motohiko Yoshimura[1] & Koji Yoshimura[1]*

^{229m}Th - a low energy metastable isomer with applications for quantum computing and atomic clocks of unprecedented accuracy (nuclear transition vs. Cs electronic transition)

Seiferle, B. *et al. Nature* **2019,** 573, 243

Masuda, T. e*t al. Nature* **2019**, *573*, 238

Notable Nuclear Isomers: ^{229m}Th

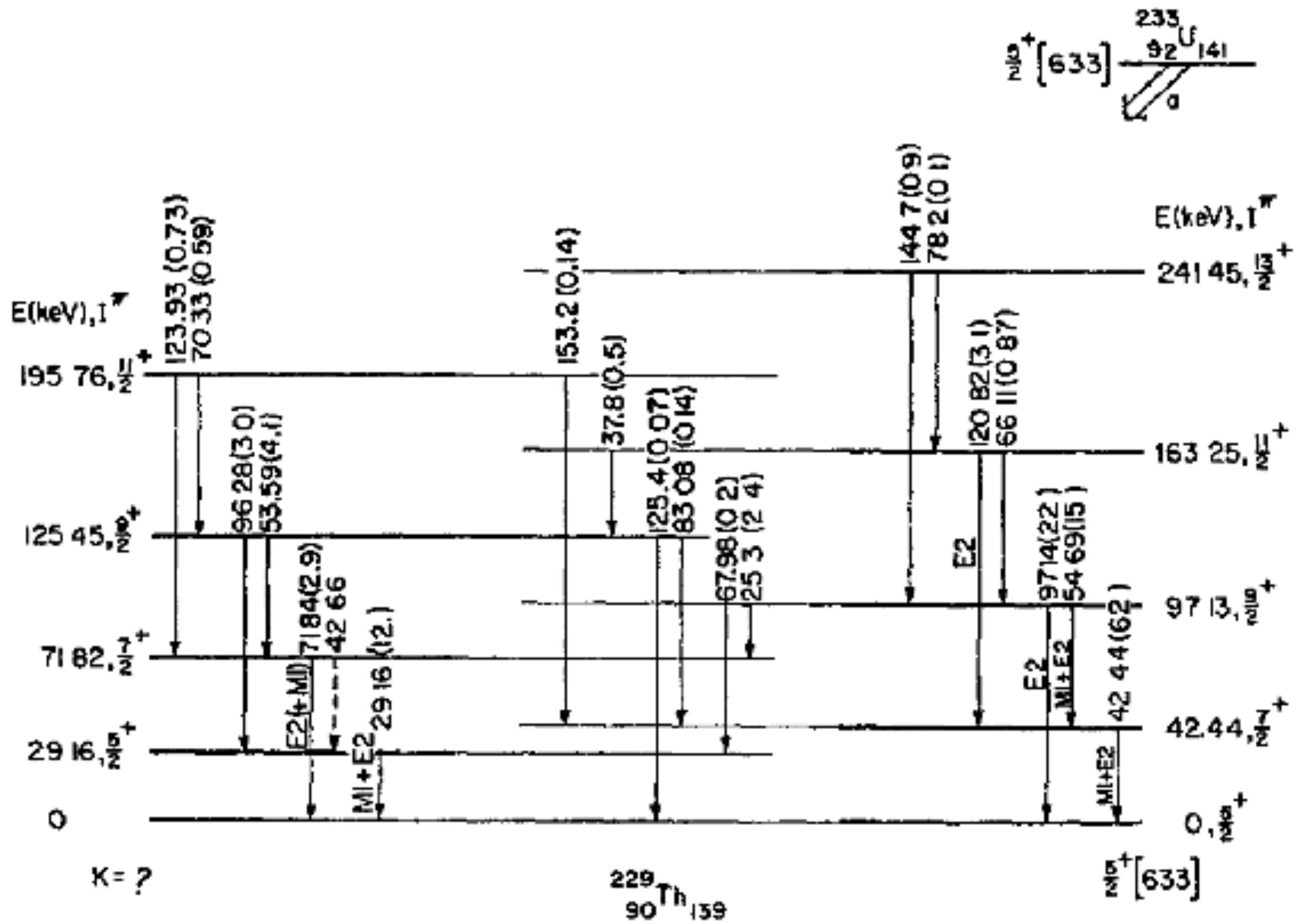


Fig. 6. Partial level scheme of ^{229}Th showing the members of the two lowest lying positive-parity bands and their associated γ-ray transitions. Although the K-value of the band indicated at the left is shown as questionable, the reasoning presented in the text strongly suggests that this band is in fact built on the $\frac{3}{2}^+$[631] Nilsson state and that the $I^\pi = \frac{3}{2}^+$ band head is located quite near to the ground state

The lowest of these bands is “shown from indirect evidence” to be within 0.1 keV of the ground state

Kroger, L.A.; Reich, C. W. *Nucl. Phys. A* **1976**, *259*, 29

Notable Nuclear Isomers: ^{229m}*Th*

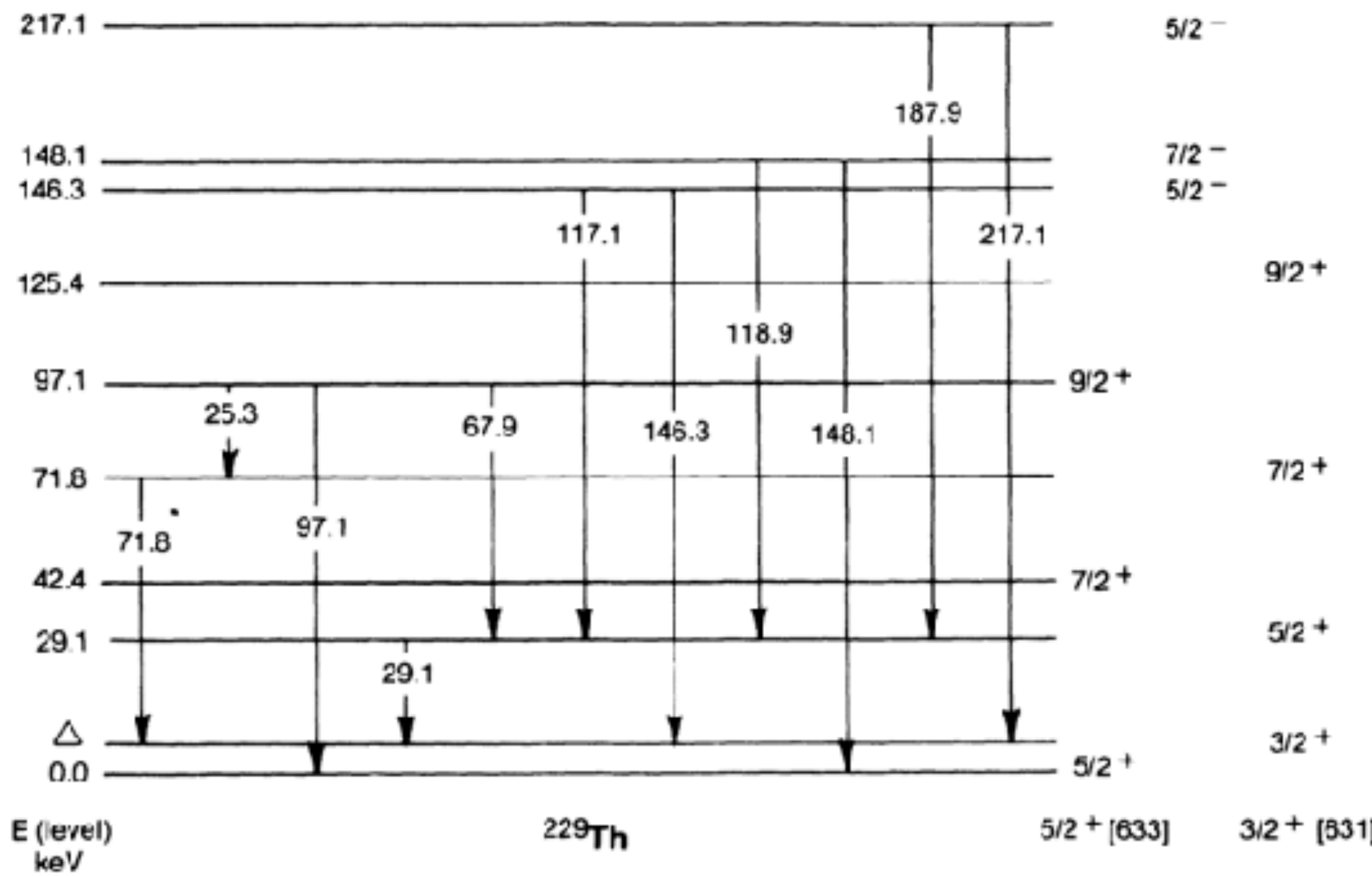


FIG. 1. Partial level scheme of ^{229}Th, showing those γ-ray transitions whose energy values were used in determining the energy separation Δ of the $\frac{5}{2}^+[633]$ and $\frac{3}{2}^+[631]$ bandheads.

3 separate indirect easurements afforded a band gap of:

$$\Delta_1 = -0.003 \pm 0.005 \text{ keV},$$

$$\Delta_2 = -0.001 \pm 0.006 \text{ keV},$$

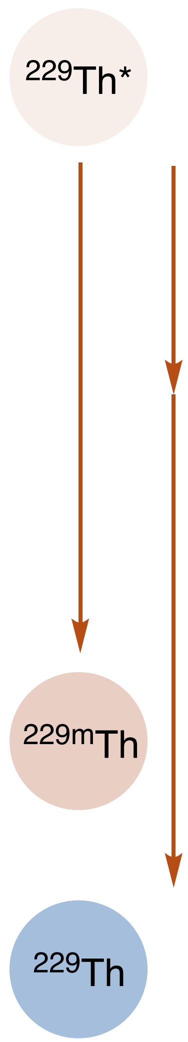
$$\Delta_3 = +0.002 \pm 0.008 \text{ keV}.$$

The group concluded that the difference between the ground and excited isomeric state was <10 eV
Instrumentation was nolonger accurate enough to determine which state was the ground state

Reich, C. W.; Helmer, R. G. *Phys. Rev. Lett.* **1990**, *64*, 271

Notable Nuclear Isomers: ^{229m}Th

Subsequent studies throughout the early 2000's, enabled by improvements in gamma ray spectoscopy, determined the isomer to be 7.8 ± 0.5 eV above the ground state



Beck, B. R. *et al*. *Phys. Rev. Lett.* **2007** *98,* 142501

Notable Nuclear Isomers: ^{229m}Th

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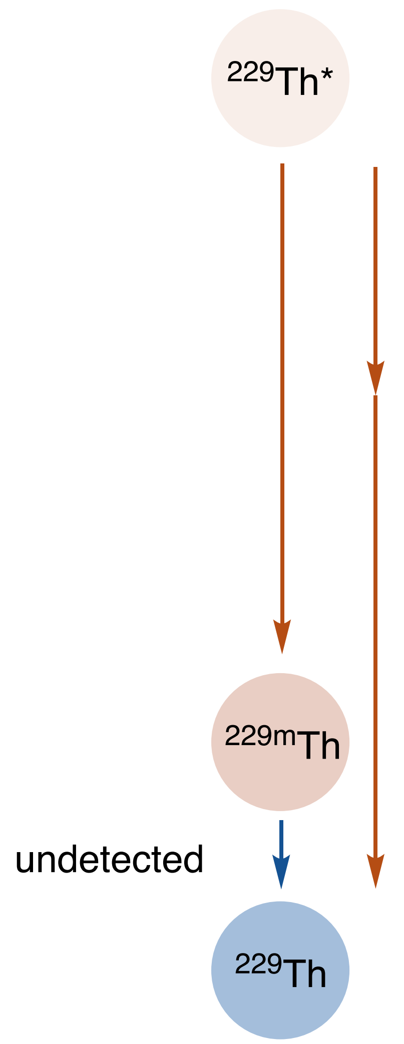

No direct observation of the decay had yet been observed

Beck, B. R. *et al*. *Phys. Rev. Lett.* **2007** *98,* 142501

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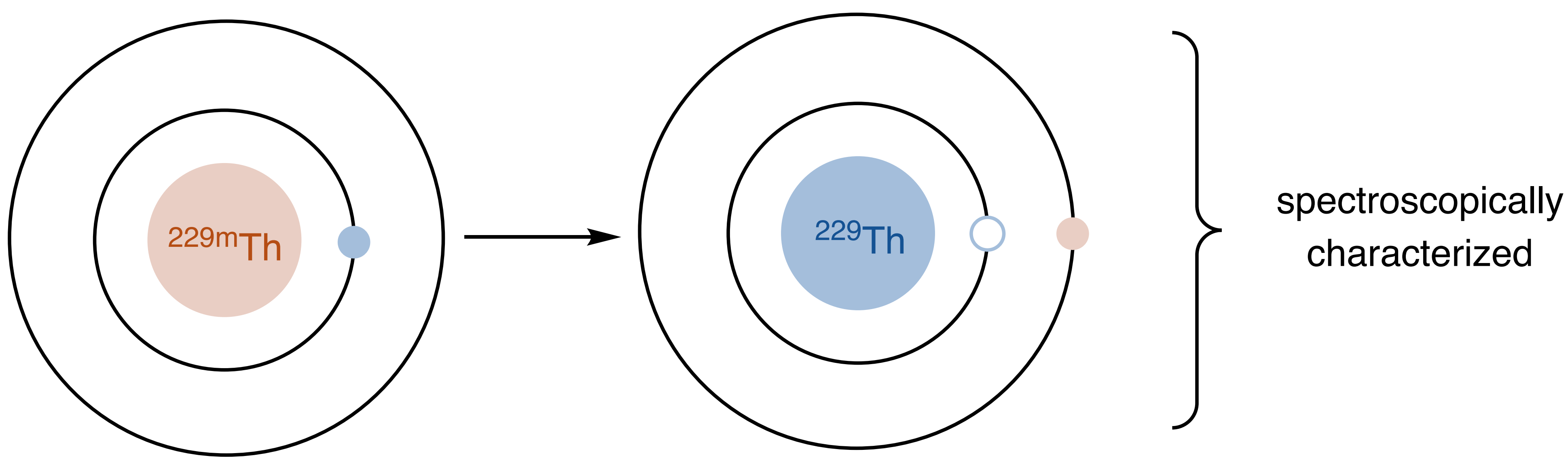
https://doi.org/10.1038/s41586-019-1533-4

Energy of the ^{229}Th nuclear clock transition

Benedict Seiferle[1]*, Lars von der Wense[1], Pavlo V. Bilous[2], Ines Amersdorffer[1], Christoph Lemell[3], Florian Libisch[3], Simon Stellmer[4], Thorsten Schumm[5], Christoph E. Düllmann[6,7,8], Adriana Pálffy[2] & Peter G. Thirolf[1]



Accurate calculation of the metastable state: 149.7 ± 3 nm

Seiferle, B. *et al. Nature* **2019,** 573, 243

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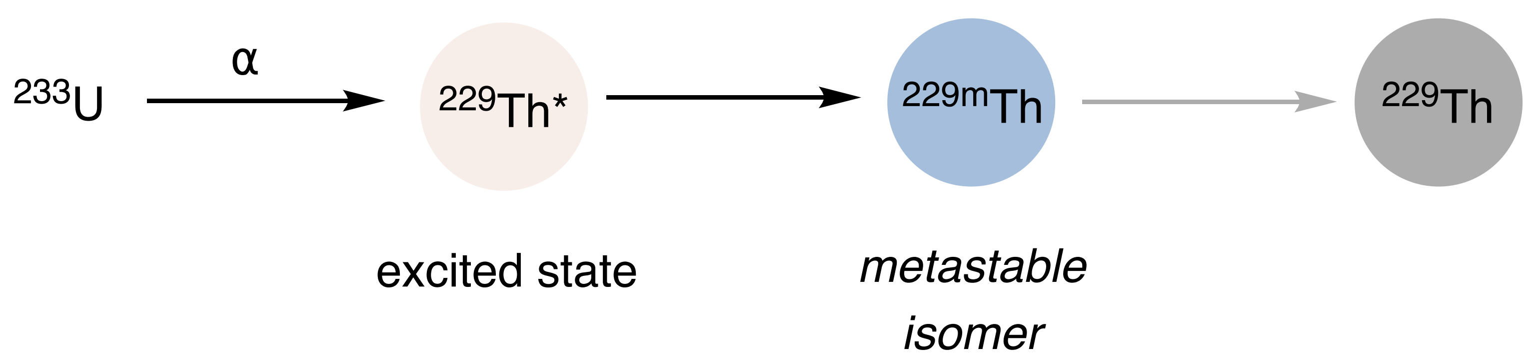
https://doi.org/10.1038/s41586-019-1542-3

X-ray pumping of the ^{229}Th nuclear clock isomer

Takahiko Masuda[1], Akihiro Yoshimi[1], Akira Fujieda[1], Hiroyuki Fujimoto[2], Hiromitsu Haba[3], Hideaki Hara[1], Takahiro Hiraki[1], Hiroyuki Kaino[1], Yoshitaka Kasamatsu[4], Shinji Kitao[5], Kenji Konashi[6], Yuki Miyamoto[1], Koichi Okai[1], Sho Okubo[1], Noboru Sasao[1]*, Makoto Seto[5], Thorsten Schumm[7], Yudai Shigekawa[4], Kenta Suzuki[1], Simon Stellmer[7,10], Kenji Tamasaku[8], Satoshi Uetake[1], Makoto Watanabe[6], Tsukasa Watanabe[2], Yuki Yasuda[4], Atsushi Yamaguchi[3], Yoshitaka Yoda[9], Takuya Yokokita[3], Motohiko Yoshimura[1] & Koji Yoshimura[1]*



Masuda, T. e*t al. Nature* **2019**, *573*, 238

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https://doi.org/10.1038/s41586-019-1542-3

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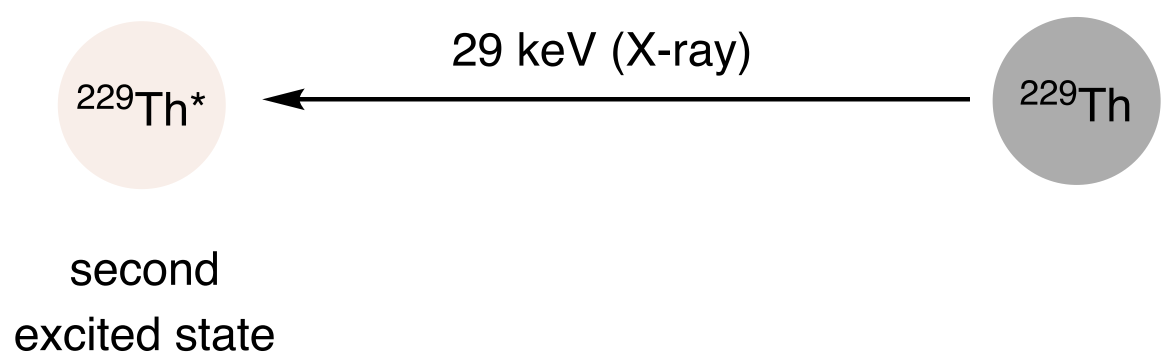

Masuda, T. e*t al. Nature* **2019**, *573*, 238

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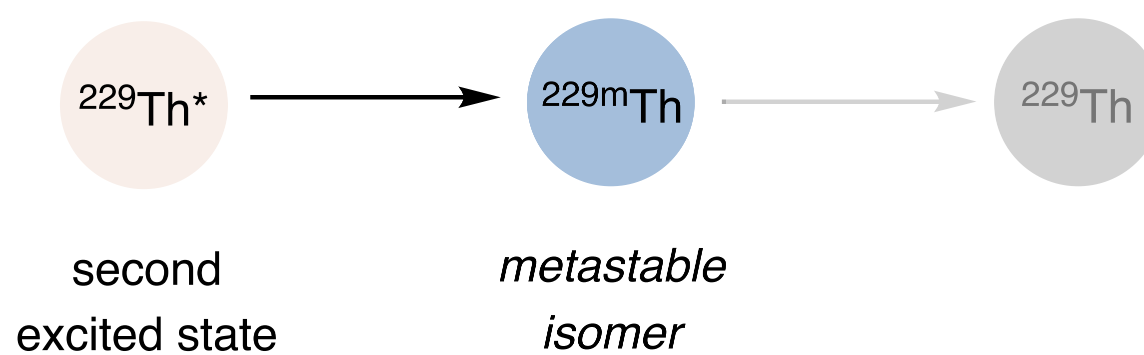

Masuda, T. e*t al. Nature* **2019**, *573*, 238