The illogical nature of chemical nomenclature

by Sophia

von Hippel, EMT, U Arizona
Chemistry Major

Our building blocks

Protons

⊕ or H^+

Our building blocks

Protons

(+) or H^+

neutrons

(n)

Our building blocks

Protons

(+) or H^+

neutrons

(n)

electrons

(−) or e^-

or •

Our building blocks

Protons

⊕ or H^+

Neutrons

(n)

electrons

⊖ or e^-

or •

atom - smallest unit of matter that forms a chemical element; a combination of protons, neutrons, and electrons

element -

A type of atom. E.g., the element Hydrogen is the atom that has only one proton.

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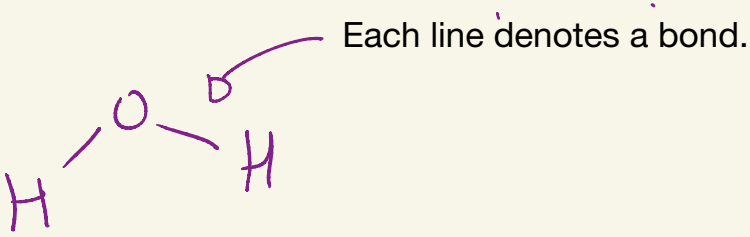
molecule – 2+ atoms bonded to one another. E.g., water = H_2O



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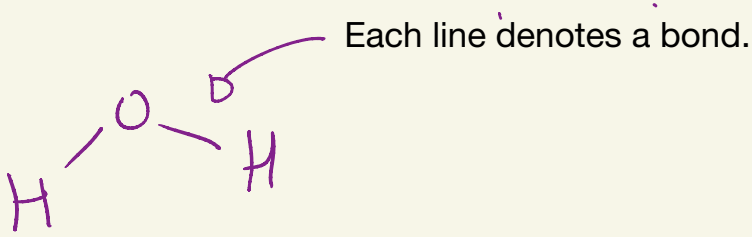


Isomers –

Atoms of the same elemental ID with differing molecular masses. Also, molecules w/ the same molecular formula but differences in conformation, stereochemistry, or mass.

For example, Hydrogen and Deuterium.

H has 1 proton

D has 1 proton and 1 neu Tron

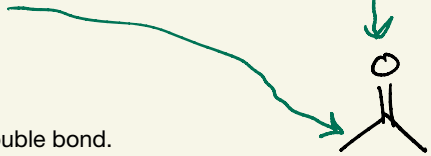
MW = $\frac{1\ g}{mol}$

MW = $\frac{2\ g}{mol}$

How are molecules represented on paper?

A line is a bond

All atoms other than Carbon and Hydrogen are drawn in.



2 lines form a double bond.

3 lines form a triple bond.

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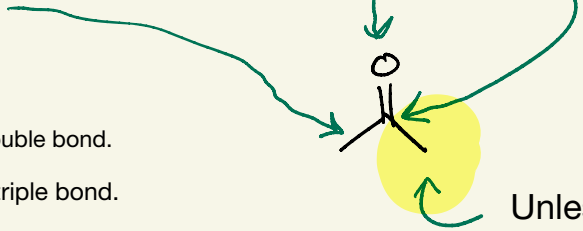

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Unless otherwise stated, all Carbon atoms have 4 bonds. One bond is already shown here, so three bonds to Hydrogens are implied.

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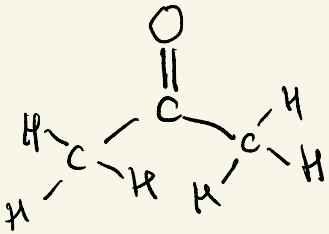

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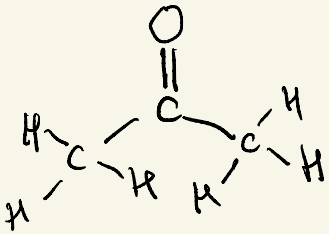


We also draw charges

And valence electrons

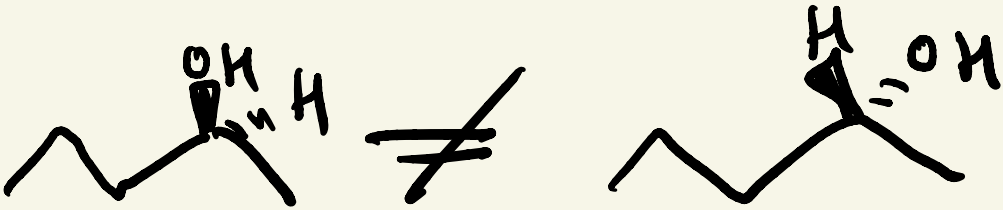
A note on stereochemistry:

Wedges come out of the page

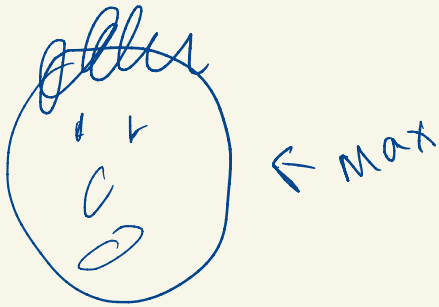
Dashes go into the page

Wedges and dashes are only used at chiral centers, which have handedness.

This is how we differentiate stereoisomers.



Max: “So Sophia, once I’ve diagrammed a molecule, how do I know what to call it, so that other researchers will unambiguously know what I am talking about?



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Easy-Peasy Lemon-Squeezy! Simply follow the rules of the IUPAC :).

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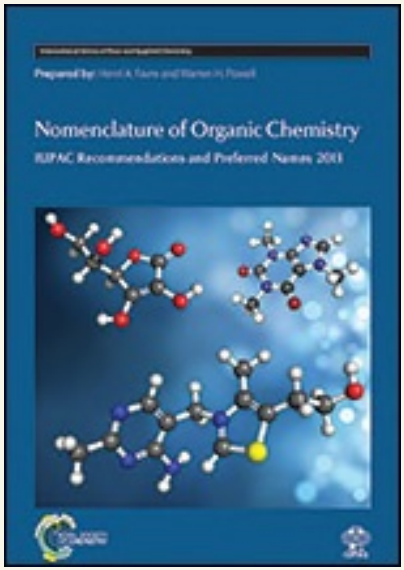

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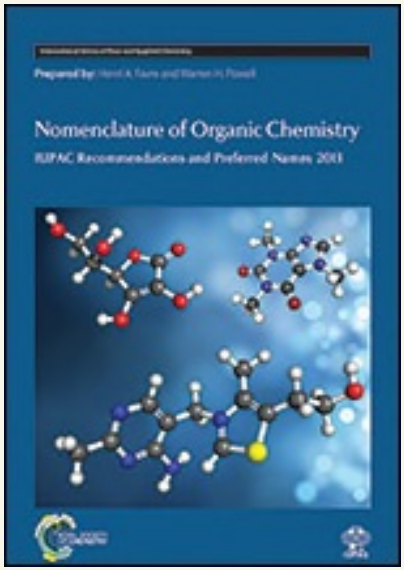

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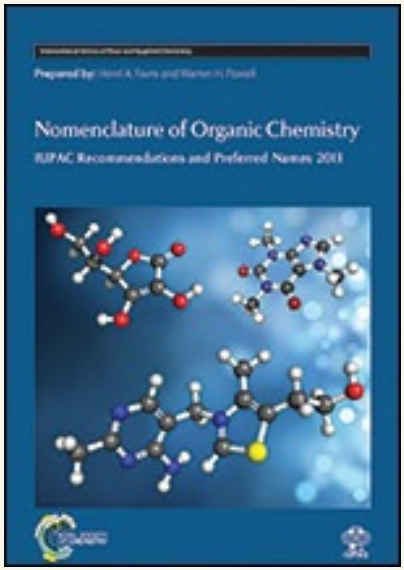

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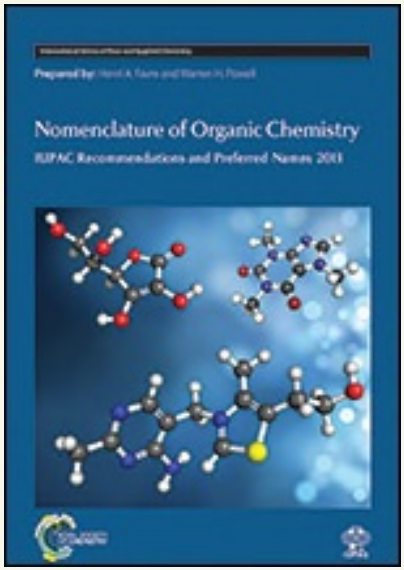

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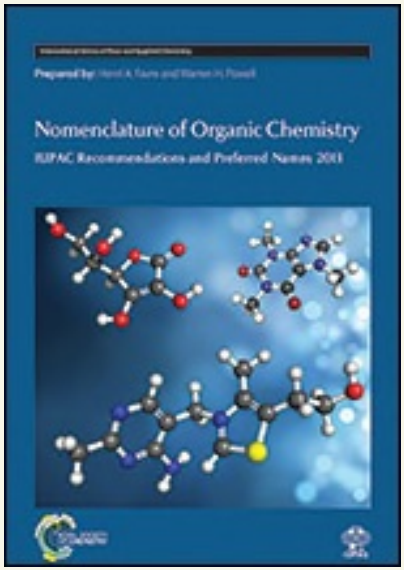

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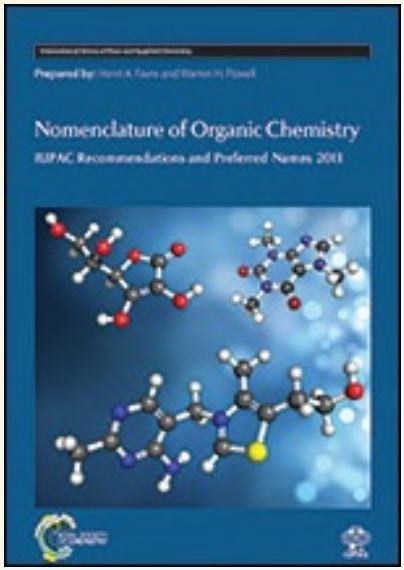

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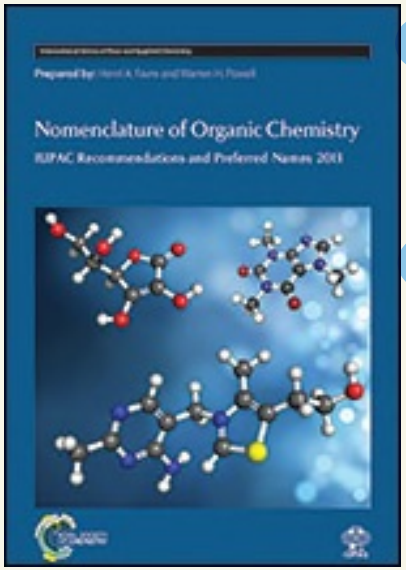

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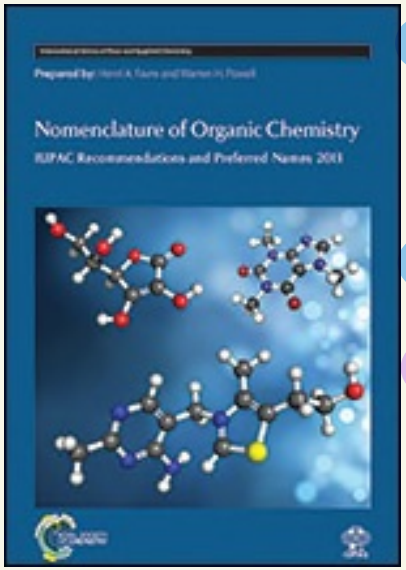

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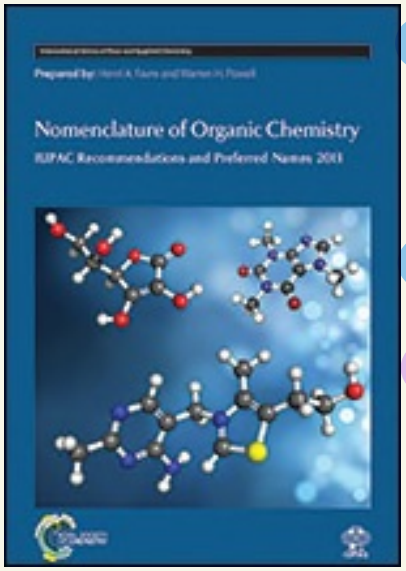

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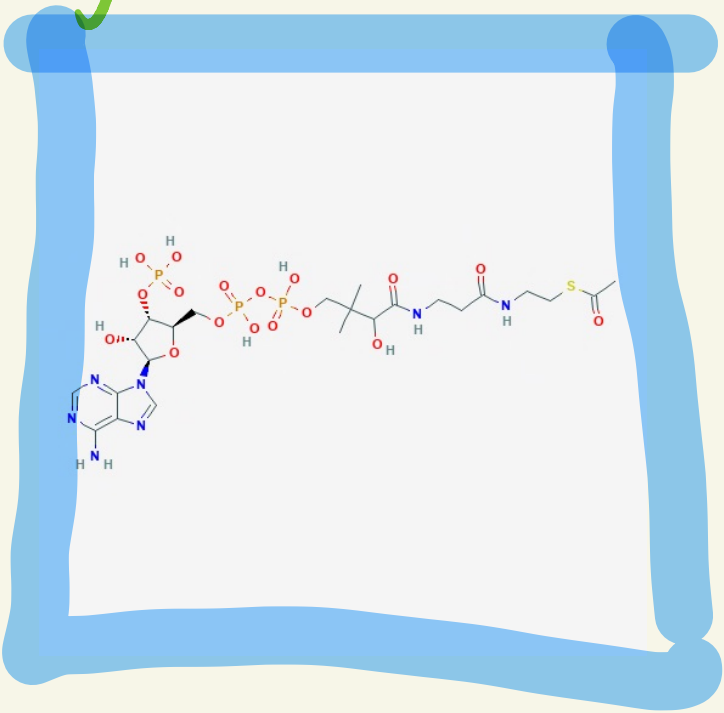
Let's take an example,

Acetyl-CoA



Why do we care?

Acetyl-CoA participates in:

- The citric acid cycle
- Cellular respiration
- Fatty acid metabolism
- Steroid synthesis
- Synthesis of the neurotransmitter Acetylcholine
- Melatonin synthesis
- etc.

So what is the official IUPAC name for Acetyl-CoA?

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Max, a chemist

thinking...

thinking...

thinking...

not making any progress whatsoever...

So what is the official IUPAC name for Acetyl-CoA?

S-[2-[3-[[4-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-4-hydroxy-3-phosphonooxyoxolan-2-yl]methoxy-hydroxyphosphoryl]oxy-hydroxyphosphoryl]oxy-2-hydroxy-3,3-dimethylbutanoyl]amino]propanoylamino]ethyl] ethanethioate

Human proteins can be up to 3700 times the size of Acetyl-CoA.

The number of possible molecules is bound only by the quantity of matter available in the universe.

Clearly, there is a reason people ignore the rules, and just call it “Acetyl-CoA”.

Question: *How can we communicate the identity of molecules in a universally readable way?*

Desirable Properties:

- When you read the name, you know what it is. No need to look it up.

- Either there is only 1 way to name something, or if there are multiple ways, then it is easy to compute all the possible names of a thing.

- It is easy to map from a name to a diagram.

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- Very large molecules could be named efficiently. E.g., if name-size was logarithmic in molecule-size.