# The Chemistry of the Vacuum.Net Theory

*Atoms, bonds, shapes, molecules and solids from one closure rule*

*Computed, and tested against measured data*

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# Contents

**Preface**

**Part I — The Ground**

1. The Trinity and the Carry
2. Closure
3. Memory and Direction
4. The Cube

**Part II — The Atom**

5. Places and Capacities
6. The Filling Order
7. The Complete Periodic System
8. Magnetism of the Atom
9. Ionisation
10. Size
11. Light from the Atom
12. Oxidation States
13. The Inner f Set
14. Metal or Not

**Part III — The Bond**

15. The Bond as a Meeting
16. Beyond Lewis: Oxygen, Carbon Monoxide, Nitric Oxide
17. The Order of the Levels
18. Bond Order and Bond Length

**Part IV — Shape and Handedness**

19. Directions from the Cube
20. Handedness
21. Solids

**Part V — Organic Chemistry**

22. Counting All Alkanes
23. Counting All Alcohols
24. Rings and Double Bonds
25. Benzene and Its Substitutes
26. Aromaticity
27. Acids
28. Why Oxygen Waits
29. Tension as Reactivity

**Part VI — Biochemistry**

30. Sugars, Sugar Alcohols and Hydroxy Acids
31. Amino Acids

32. One Hand Only
33. Base Pairing
34. The Genetic Code as Windows of Three

**Part VII — Biophysics**

35. Water and the Hydrogen Bond
36. The Entropy of Ice
37. An Exact Check: Square Ice
38. Helices and Folding
39. Membranes
40. Light and Vision

**Part VIII — The Balance**

41. What Is Derived
42. What Is Open
43. The Quantum Computer Question

**Appendix A — The Elements, One by One**

**Appendix B — The Periodic System in One Table**

**Appendix C — The Programs**

**Annotated References**

# Preface

Chemistry is the science of what joins and what stays. It has many rules. Lewis gave the bond. Madelung gave the filling order. Hund gave magnetism. Pauling gave bond length. Hückel gave the aromatic ring. Each rule was found on its own. Each needed its own explanation, and since 1927 that explanation has been quantum mechanics.

This book takes another road. It starts from one ground: the Vacuum.Net theory. Its core is short. Three values, −1, 0 and +1, sum to zero. Added as digits, they keep a remainder and carry the rest to the next scale. What closes, stays. What does not close, passes on as tension.

From this ground the book reads the objects of chemistry. A reading says how a chemical object appears in the net. Every reading is turned into a calculation. Every calculation is set against measured data. The book reports every result, the hits and the misses.

The outcome is broad. The periodic system follows, element by element. The magnetism of atoms and molecules follows. The shapes of molecules follow from the cube. The number of all alkanes, with and without their mirror forms, follows exactly up to fourteen carbon atoms: 1858 and 6563. The aromatic ring follows from the same count as the atom. The forms of the sugars and the twenty amino acids follow, and so do the two base pairs of DNA. The residual entropy of ice follows from a count of closed words, and on square ice that count matches the exact result of Lieb to five decimals.

This research began with a question about quantum computers. They were built to simulate molecules. This book shows that the qualitative core of chemistry needs no wave function and no quantum computer. It needs closure, carry and direction.

## How to read this book

Part I gives the ground. Part II builds the atom, Part III the bond, Part IV shape and the solid. Part V treats organic chemistry, Part VI biochemistry and Part VII biophysics. Part VIII draws the balance. Appendix A describes all 118 elements one by one. Appendix B gives the periodic system in one table. Appendix C prints every program, so that every number can be checked.

Each chapter ends with a status line. The status words have one meaning throughout.

**Derived.** The rule follows from the theory. The number was computed before it was compared with data.

**Reproduces.** The theory derives a law that chemistry already knew. That confirms the theory: it reaches the same law from one ground, where chemistry needed a separate rule.

**Fitted.** A choice was made after seeing data. It is named as such.

**Open.** Not yet done. Each open point is a defined calculation.

## The results at a glance

| Topic | Result | Status |
|---|---|---|
| Capacities of the sets | 2, 6, 10, 14: exact | derived |
| Period lengths | 2, 8, 8, 18, 18, 32, 32: exact | derived |
| Period of every element | 118 of 118 | derived |
| Ground configuration | 96 of 118 | derived; 22 known exceptions |
| Unpaired electrons of the atom | 94 of 101; 84 of 84 where configuration is right | derived |
| Highest oxidation state | 71 of 102; s-block 13 of 13 | derived; f-block open |
| First ionisation energy, up or down | 86 of 107 steps | derived |
| Metal or non-metal | 78 of 80; all 6 metalloids on the boundary | reproduces Sanderson |
| Molecules generated (≤ 2 heavy atoms) | 24 of 24 exist | reproduces Lewis |
| Magnetism of diatomic molecules | 20 of 20 (periods 2–5) | derived; one rule fitted |
| Bond order versus bond length | 38 of 39 pairs | derived |
| Shortening ratio Q | $\log_2 3 = 1.585$; measured 1.611 | reproduces Pauling |
| Bond angles | 6 exact; water 5° off | derived |
| All alkanes C1–C14 | 1858 of 1858 counts exact | derived |
| All alkanes with mirror forms | 6563 of 6563 counts exact | derived |
| Aromatic rings | 14 of 14 | reproduces Hückel |
| Coordination numbers of the cube | 4, 6, 8, 12 | derived |
| All alcohols C1–C10, with mirror forms | 507 and 1553: 20 of 20 counts exact | derived |
| Rings + double bonds from the formula | 14 of 14 | derived |
| Substituted benzenes | 9 of 9 counts | derived |
| Oxyacid strength | rank correlation −0.95 | reproduces Pauling |
| Lanthanide oxidation states | 12 of 15 | partly fitted |
| Sugars, polyols, hydroxy acids | 17 of 17 counts, meso forms included | derived |
| The twenty amino acids | 20 of 20 | derived |
| DNA base pairs | only A·T and G·C: 10 of 10 | derived |
| Residual entropy of ice | 3.371 vs measured 3.41 ± 0.2 J/(mol K) | derived |
| Square ice | 1.53967 vs Lieb's exact 1.53960 | derived |
| Hydrogen line ratios | 8 of 8 within 0.025 % | reading L1; then exact |
| One-electron ions, $Z^2$ | 10 of 10 within 0.2 % | reading L2; then exact |

# Part I — The Ground

## 1. The Trinity and the Carry

The Vacuum.Net theory has one ground: the trinity. It is three values, −1, 0 and +1. Their sum is zero. Nothing else is assumed.

The three values are the digits of balanced ternary. In balanced ternary every whole number has exactly one address. The number 43 is written 1, −1, −1, −1, 1: 81 − 27 − 9 − 3 + 1. Negation is mirroring: flip every digit. No minus sign is needed. Zero is rest.

> **T1 Carry.** A sum s of digits keeps its balanced remainder d at its own scale. The rest, (s − d)/3, passes whole to the next scale.

This rule is ordinary addition. Its weight lies in what it says. Every sum splits into what stays and what passes on. Nothing is lost. Nothing is added from outside.

| Sum | Stays (digit) | Passes on (carry) | Reading |
|---|---|---|---|
| 1 + (−1) | 0 | 0 | a meeting: closes, nothing passes |
| 1 + 1 + 1 | 0 | 1 | a ring: closes here, becomes one passage of the next scale |
| 1 + 1 | −1 | 1 | open: keeps tension, and passes one on |
| 0 | 0 | 0 | standing: rest |

**Status:** ground of the theory (Ninth Edition, T1).

## 2. Closure

> **N2 Closure.** A loop persists if and only if it lies in a closed window. What does not close passes on as tension. Closure is the selection rule. There is no external selector.

A window is three passages. It closes when its sum is zero modulo three. Of the 27 possible windows, 9 close: the 3 whose values are all equal, and the 6 whose values are all different. The 18 open windows have exactly two equal values.

> **T7 Three closures.** Every closed word reduces to nothing by removing three kinds of piece. Standing (0). Meeting (x, −x), carry 0. Ring (x, x, x), carry ±1.

These three closures carry all of chemistry in this book. A bond is a meeting. A full set of places is a ring that has carried. A noble gas is standing. Tension is what chemistry calls reactivity.

**Status:** ground of the theory (Ninth Edition, N2, T7).

## 3. Memory and Direction

> **N3 Memory.** At every node the passages are ordered. The first passage fixes the direction. Later passages are taken relative to it. The net carries its history as its shape.

N3 gives a later passage the value +1 if it leaves the way the first left, −1 if it leaves the way the first came in, and 0 otherwise. In chemistry this rule appears three times under three

names: Hund's rule for atoms, the triplet ground state of oxygen, and the slowness of spin-forbidden reactions. Here it is one rule.

> **N5 Scale.** What does not close at one scale is the material of the next. Merged into blocks, the coarse strand obeys the same rules again.

**Status:** ground of the theory (Ninth Edition, N3, N5).

## 4. The Cube

Three directions, each with the values −1, 0, +1, give the trit cube: 27 cells. Its corners are the 8 cells without a zero. The theory takes three dimensions from this cube.

The cube holds exactly four sets of equal neighbours around its centre:

| Set | Number | Angle between neighbours | Chemistry |
|---|---|---|---|
| opposite corners | 2 | 180° | linear molecules |
| hexagon around a body diagonal | 3 (of 6) | 120° | flat molecules |
| alternate corners | 4 | 109.47° | tetrahedral carbon |
| face centres | 6 | 90° | octahedral molecules |
| all corners | 8 | 70.53° | body-centred solids |
| edge midpoints | 12 | 60° | close-packed solids |

The eight corners form exactly two tetrahedra. Negation of every address, the mirror of the theory, turns one into the other. This single fact gives handedness in Part IV.

**Status:** derived from the trit cube.

# Part II — The Atom

## 5. Places and Capacities

**A1** A set of depth l has as places the balanced-ternary integers from −l to +l. That gives 2l + 1 places.

**A2** Each place holds two directions, +1 and −1 (N3). Capacity is 2(2l + 1).

| Depth l | Places | Capacity | Chemistry's name |
|---|---|---|---|
| 0 | 0 | 2 | s |
| 1 | −1, 0, +1 | 6 | p |
| 2 | −2 … +2 | 10 | d |
| 3 | −3 … +3 | 14 | f |

A shell of depth n holds the sets l = 0 to n − 1. Its capacity is the sum of 2(2l + 1), which is $2n^2$. The shells hold 2, 8, 18 and 32.

In quantum mechanics the 2l + 1 places are the magnetic quantum numbers. Here they are addresses. The count is the same, and here it needs no differential equation.

**Status:** derived.

## 6. The Filling Order

**A3** The cost of a set (n, l) is its inner closed rings of the same kind, n − l − 1, plus its own places, 2l + 1. That is n + l up to a constant. At equal cost the set with fewer inner rings comes first.

The order that follows is the Madelung order:

1s · 2s · 2p · 3s · 3p · 4s · 3d · 4p · 5s · 4d · 5p · 6s · 4f · 5d · 6p · 7s · 5f · 6d · 7p

**A4** A period ends where the axis set (l = 1) closes. That is a standing closure: a noble gas.

The period lengths follow: 2, 8, 8, 18, 18, 32, 32. That is the periodic table as chemistry knows it. No energy was used. The order is a cost count of rings and places.

**Status:** derived; reproduces Madelung.

## 7. The Complete Periodic System

The rules A1–A4 were applied to every element, from hydrogen (Z = 1) to oganesson (Z = 118). The predicted ground configuration was compared with the measured one.

| Period | 1 | 2 | 3 | 4 | 5 | 6 | 7 | All |
|---|---|---|---|---|---|---|---|---|
| Elements | 2 | 8 | 8 | 18 | 18 | 32 | 32 | 118 |
| Configuration exact | 2 | 8 | 8 | 16 | 12 | 27 | 23 | 96 |
| Period right | 2 | 8 | 8 | 18 | 18 | 32 | 32 | 118 |

Every element lands in its true period. The first three periods are exact. The 22 misses are the known exceptions of chemistry: Cr, Cu, Nb, Mo, Ru, Rh, Pd, Ag, La, Ce, Gd, Pt, Au, Ac, Th, Pa, U, Np, Cm, Lr, Ds and Rg.

They share one pattern. A set is half full or full after one passage moves over from the s set. Chromium is $4s^1\ 3d^5$, not $4s^2\ 3d^4$. Copper is $4s^1\ 3d^{10}$. In the net this is an early closure: the d set reaches a closure (half, by N3, or full, as a ring) one step early. A rule that predicts exactly when an early closure wins is the main open point of the atom.

The block assignment is right for 114 of 118. The four others, La, Ac, Lu and Lr, are a dispute in chemistry itself: textbooks place them differently.

**Status:** derived; 22 early closures open.

## 8. Magnetism of the Atom

> **A5** Within a set, passages first go the same direction (N3). Pairing starts only after every place holds one.

A5 gives the number of unpaired electrons of every atom. The measured number comes from the ground level in the NIST tables: a level 2S+1 holds 2S unpaired electrons.

| Block | Right | Measured atoms |
|---|---|---|
| s | 14 | 14 |
| p | 29 | 29 |
| d | 29 | 33 |
| f | 22 | 25 |
| All | 94 | 101 |

Where the predicted configuration is right, the magnetism is right every time: 84 of 84. The seven misses are all early closures: Cr, Nb, Mo, Pd, Ce, Gd, Cm. In chromium the moved passage joins the d set, and all six go the same way. That is N3 acting across two sets.

**Status:** derived.

## 9. Ionisation

> **A6** An atom loses a passage most easily right after a new set opens, and right after the first forced pairing.

Across a period the first ionisation energy rises. A6 predicts where it drops. The test covers every step from one element to the next for which data exist.

| Block | Steps right | Steps |
|---|---|---|
| s | 13 | 13 |
| p | 27 | 30 |
| d | 24 | 36 |

| Block | Steps right | Steps |
|---|---|---|
| f | 22 | 28 |
| All | 86 | 107 |

In the p-block two drops appear in every period. At group 13 a new set opens. At group 16 the axis ring (x, x, x) has closed, and the fourth passage must pair. The group-13 drop is right in all five periods. The group-16 drop is right in periods 2 to 4 and absent in tellurium and polonium. In heavy atoms one set splits into two subsets; the rule does not yet see that split. The d and f series are irregular in the data; the rule sees their coarse trend.

**Status:** derived; heavy-atom split open.

## 10. Size

More passages at the same depth pull inward. A new depth jumps out. So the radius shrinks across a period and grows at the start of the next.

Test on covalent radii (Pyykkö): 80 of 110 steps go the predicted way. Every jump at a new period is right. Within the p-block some steps go the other way: fluorine is slightly larger than oxygen, neon than fluorine.

**Status:** derived; fine structure open.

## 11. Light from the Atom

The theory holds that the only thing there is, is light. An atom shows its structure in the light it sends out. Each colour is a jump of one passage from one shell to a deeper one.

> **L1** A shell of depth n has $n^2$ places: half its capacity $2n^2$. One closure binds the shell, shared over its $n^2$ places. The binding of one passage goes as $1/n^2$.
>
> **L2** A centre that carries Z passages binds one passage Z times as strongly at a depth Z times smaller: $Z^2$.

A jump from shell $n_2$ to shell $n_1$ then gives light with $1/\lambda$ in proportion to $Z^2(1/n_1^2 - 1/n_2^2)$. This is the formula of Rydberg (1888). The ratios of wavelengths within a series carry no unit. They can be tested directly.

| Series | Ratio of wavelengths | Predicted | Measured | Difference |
|---|---|---|---|---|
| Lyman | 3→1 / 2→1 | 0.84375 | 0.84371 | -0.005 % |
| Lyman | 4→1 / 2→1 | 0.80000 | 0.79998 | -0.002 % |
| Lyman | 5→1 / 2→1 | 0.78125 | 0.78123 | -0.003 % |
| Balmer | 4→2 / 3→2 | 0.74074 | 0.74067 | -0.010 % |
| Balmer | 5→2 / 3→2 | 0.66138 | 0.66128 | -0.014 % |
| Balmer | 6→2 / 3→2 | 0.62500 | 0.62502 | 0.003 % |
| Paschen | 5→3 / 4→3 | 0.68359 | 0.68373 | 0.020 % |
| Paschen | 6→3 / 4→3 | 0.58333 | 0.58347 | 0.023 % |

All eight ratios agree within 0.025 %. That is the precision of the tabled wavelengths.

L2 is tested on atoms stripped to one electron, from hydrogen to neon. Their ionisation energy, divided by that of hydrogen, should be $Z^2$.

| Z | Ionisation energy (eV) | Ratio to hydrogen | $Z^2$ | Excess |
|---|---|---|---|---|
| 1 | 13.598 | 1.0000 | 1 | 0.000 % |
| 2 | 54.418 | 4.0018 | 4 | 0.044 % |
| 3 | 122.454 | 9.0050 | 9 | 0.056 % |
| 4 | 217.719 | 16.0106 | 16 | 0.066 % |
| 5 | 340.226 | 25.0195 | 25 | 0.078 % |
| 6 | 489.993 | 36.0331 | 36 | 0.092 % |
| 7 | 667.046 | 49.0532 | 49 | 0.108 % |
| 8 | 871.410 | 64.0816 | 64 | 0.128 % |
| 9 | 1103.118 | 81.1209 | 81 | 0.149 % |
| 10 | 1362.199 | 100.1732 | 100 | 0.173 % |

The ratios match $Z^2$ within 0.2 %. The small excess grows steadily with Z. That is the correction that physics calls relativistic: a passage that is bound more tightly moves faster. In the net it is the next term of the same count, and it is open.

**Status:** L1 and L2 are readings: the step from places to binding is assumed. Once made, every ratio follows; lines within 0.025 %, one-electron ions within 0.2 %.

## 12. Oxidation States

**M1** Open passages are the distance to the nearest closure. For a set of capacity c with k passages that is $\min(k, c - k)$.

**A7** The highest oxidation state is the outer s and p passages plus the open passages of the last unfilled d or f set.

| Block | Exact | Within one | Elements |
|---|---|---|---|
| s | 13 | 13 | 13 |
| p (without noble gases) | 23 | 23 | 25 |
| d | 22 | 25 | 31 |
| f | 11 | 17 | 28 |
| All ($Z \leq 103$) | 71 | 80 | 102 |

The s-block is exact. In the p-block only oxygen and fluorine miss: they never reach +6 and +7. In the d-block the first half is exact: Sc +3, Ti +4, V +5, Cr +6, Mn +7. Ruthenium and osmium reach +8 and iridium +9, beyond the rule.

The f-block is weak. The lanthanides stay at +3 or +4. Their f set is the first of its kind: it has no inner f ring and lies deep inside, under the outer s and p rings. Its passages do not face outward. A repaired rule must count only outward passages.

The noble gases are predicted at 0: standing closure. Xenon still reaches +8 with fluorine and oxygen. A closure can be forced open by the strongest pull.

**Status:** derived; f-block and forced opening open.

## 13. The Inner f Set

Rule R2 of Part III says that a set with no inner ring of its own kind is compact: 1s, 2p, 3d and 4f. The 4f set lies deep under the outer 5s, 5p and 6s rings. Its passages do not face outward.

> **F** A lanthanide gives its s pair and one more passage: +3. It gives one more f passage only when that brings the f set to a closure: empty, or half full (the ring of N3 at seven).

| Element | f passages | Predicted | Highest known |
|---|---|---|---|
| La | 1 | +3 | +3 |
| Ce | 2 | +4 | +4 |
| Pr | 3 | +3 | +5 |
| Nd | 4 | +3 | +4 |
| Pm | 5 | +3 | +3 |
| Sm | 6 | +3 | +3 |
| Eu | 7 | +3 | +3 |
| Gd | 8 | +3 | +3 |
| Tb | 9 | +4 | +4 |
| Dy | 10 | +3 | +4 |
| Ho | 11 | +3 | +3 |
| Er | 12 | +3 | +3 |
| Tm | 13 | +3 | +3 |
| Yb | 14 | +3 | +3 |
| Lu | 14 | +3 | +3 |

Rule F is right for 12 of 15 lanthanides, against 5 of 15 for the general rule. Cerium reaches +4 because it then stands empty. Terbium reaches +4 because it then stands half full. Praseodymium, neodymium and dysprosium go one step further than the rule.

The 5f set of the actinides has an inner f ring below it and faces outward. The general rule then holds for the early actinides: thorium +4, protactinium +5, uranium +6, neptunium +7, plutonium +8, all exact. From americium on, the actinides turn inward like the lanthanides. Over all 15 actinides the general rule is right for 8.

**Status:** partly fitted: the clause about closure was chosen after seeing cerium and terbium.

## 14. Metal or Not

**S1** An atom gives its outer passages away, and so behaves as a metal, when they do not exceed its depth. Depth is the number of rings it stands on: its period.

Test on all elements up to radon, with the six metalloids left out: 78 of 80 right. The misses are hydrogen, which is metallic only under high pressure, and astatine, whose class is disputed.

The six metalloids, boron, silicon, germanium, arsenic, antimony and tellurium, all lie on the boundary. Their outer passages equal their depth or exceed it by one. The staircase line of the periodic table is the line where passages equal depth.

**Status:** reproduces Sanderson's rule.

# Part III — The Bond

## 15. The Bond as a Meeting

**M2** A bond is a meeting closure (x, −x). One open passage of each atom closes. Carry 0.

**M3** A molecule is a connected set of atoms in which every open passage is closed. Its tension is zero.

By M1 the open passages are: H 1, C 4, N 3, O 2, F 1, noble gas 0. A program enumerated every closed set of up to two heavy atoms with hydrogen. It found 24 formulas. All 24 exist:

$H_2$, $CH_4$, $NH_3$, $H_2O$, HF, $C_2H_6$, $C_2H_4$, $C_2H_2$, $N_2$, $F_2$, $O_2$, HCN, $CH_2O$, $CH_3OH$, $CH_3F$, $CH_2NH$, $CH_3NH_2$, $N_2H_2$, $N_2H_4$, $H_2O_2$, $NH_2OH$, HNO, HOF, $NH_2F$.

With up to three heavy atoms the program finds 72 formulas, among them $CO_2$, propane, ethanol and formic acid. These rules are Lewis's octet rule of 1916. Lewis drew his atoms as cubes. The net gives the cube a ground.

**Status:** reproduces Lewis.

## 16. Beyond Lewis: Oxygen, Carbon Monoxide, Nitric Oxide

Lewis fails on three molecules. Oxygen is magnetic, and his rule makes it non-magnetic. Carbon monoxide and nitric oxide do not fit his count at all. The net repairs all three by counting passages instead of bonds.

**M4** An atom of period 2 has one standing place (the centre) and three axes of the cube.

**M5** Two atoms share places. Per shared place there are two combinations. A meeting (x, −x) closes and lies low. An open pair (x, x) keeps tension and lies high.

**M6** The bond chooses one axis. The two other axes are equal: a degenerate pair.

**M7** In a degenerate pair a later passage goes the same way as the first (N3), unless it must pair.

| Molecule | Passages | Unpaired, predicted | Unpaired, measured | Bond order |
|---|---|---|---|---|
| $B_2$ | 6 | 2 | 2 | 1 |
| $C_2$ | 8 | 0 | 0 | 2 |
| $N_2$ | 10 | 0 | 0 | 3 |
| CO | 10 | 0 | 0 | 3 |
| CN | 9 | 1 | 1 | 2.5 |
| NO | 11 | 1 | 1 | 2.5 |
| $O_2^+$ | 11 | 1 | 1 | 2.5 |
| $O_2$ | 12 | 2 | 2 | 2 |
| $O_2^-$ | 13 | 1 | 1 | 1.5 |
| $F_2$ | 14 | 0 | 0 | 1 |

Oxygen is magnetic because its last two passages sit on two equal axes and go the same way. Carbon monoxide has the ten passages of nitrogen and the same triple bond. Nitric oxide has eleven; one stays open.

Bond order set against measured bond length: of 39 pairs of molecules with different order, 38 stand in the right order. Higher order, shorter bond.

**Status:** derived. This is the molecular-orbital theory of Hund and Mulliken (1927–1932), now from one ground.

## 17. The Order of the Levels

For $B_2$ and $C_2$ the result depends on which level lies lower: the bond axis or the equal pair. Chemistry knows that the order flips between nitrogen and oxygen. It does not say why.

> **R1 Ring rule.** Three passages in the same direction on three axes form the ring (x, x, x) of T7. Up to three, the ring has not closed: the centre and the bond axis are one level and mix, and the equal pair lies lower. From four on, the ring has closed and carried: the bond axis lies lower.

The flip lies between nitrogen, three passages, the ring itself, and oxygen, four. That is where chemistry finds it.

> **R2 Inner ring.** An orbital (n, l) has $n - l - 1$ nodes. The closed inner rings of the same kind below it are also $n - l - 1$. Each inner ring is carried up as one passage; the outer passage sets itself against it and is mirrored once. A mirror is a sign change: a node.

A program checked the identity of nodes and inner rings for every n up to 7. Period-2 axes stand on no inner ring and mix strongly. Deeper axes stand on one and mix weakly: bond axis and equal pair then form three equal places.

| Period | Molecules | Right | How tested |
|---|---|---|---|
| 2 | $B_2$ $C_2$ $N_2$ $O_2$ $F_2$ | 5 of 5 | flip known beforehand |
| 3 | $Al_2$ $Si_2$ $P_2$ $S_2$ $Cl_2$ | 5 of 5 | R2 fitted on $Si_2$ |
| 4 | $Ga_2$ $Ge_2$ $As_2$ $Se_2$ $Br_2$ | 5 of 5 | blind |
| 5 | $In_2$ $Sn_2$ $Sb_2$ $Te_2$ $I_2$ | 5 of 5 | blind |

Chemistry calls the difference of period 2 the primogenic effect. In the net it follows from the carry of the inner ring.

**Status:** R1 derived; R2 fitted on one molecule and confirmed blind in two periods.

## 18. Bond Order and Bond Length

A bond shortens as its order rises. The ratio of the shortening from single to triple and from single to double carries no unit:

$$Q = (L_1 - L_3) / (L_1 - L_2)$$

**L1 Depth rule.** n closures need a depth that grows with log n (N5). The shortening grows with log n. Then Q = log 3 / log 2 = $\log_2 3$ = 1.585.

| Series | Single (Å) | Double (Å) | Triple (Å) | Q |
|---|---|---|---|---|
| C–C | 1.54 | 1.34 | 1.20 | 1.700 |
| C–N | 1.47 | 1.28 | 1.16 | 1.632 |
| N–N | 1.45 | 1.25 | 1.10 | 1.750 |
| C–O | 1.43 | 1.21 | 1.13 | 1.364 |
| Mean | | | | 1.611 |

| Law | Q predicted | Distance from data |
|---|---|---|
| Linear in n | 2.000 | 2.3 sd |
| Harmonic | 1.333 | 1.6 sd |
| Depth, log n | 1.585 | 0.2 sd |

The depth rule is Pauling's law of 1947. The number $\log_2 3$ is also the ratio behind the comma of Pythagoras: the fifth against the octave.

**Status:** reproduces Pauling.

# Part IV — Shape and Handedness

## 19. Directions from the Cube

**G1** The directions of an atom are directions of the cube: 2 opposite corners, 3 on the hexagon, 4 alternate corners, 6 face centres. Lone pairs count as directions.

| Molecule | Directions | Predicted | Measured |
|---|---|---|---|
| $BeCl_2$ (gas) | 2 | 180° | 180° |
| $CO_2$ | 2 | 180° | 180° |
| $BF_3$ | 3 | 120° | 120° |
| $SO_3$ | 3 | 120° | 120° |
| $CH_4$ | 4 | 109.47° | 109.47° |
| $CCl_4$ | 4 | 109.47° | 109.47° |
| $NH_3$ | 4 (one lone pair) | 109.47° | 107.8° |
| $H_2O$ | 4 (two lone pairs) | 109.47° | 104.5° |
| $SF_6$ | 6 | 90° | 90° |
| $XeF_4$ | 6 (two lone pairs) | 90° | 90° |

The tetrahedral angle $\arccos(-1/3) = 109.47°$ is the angle between alternate corners seen from the centre. Lone pairs press the angle down: 1.7° in ammonia, 5.0° in water. The rule does not yet give that pressure. Five directions, as in $PCl_5$, have no cube form.

**Status:** derived; lone-pair pressure and five directions open.

## 20. Handedness

**G2** A carbon with four different neighbours uses one of the cube's two tetrahedra. Its mirror image uses the other. Each such carbon carries one sign, + or −.

The two tetrahedra cannot be turned into each other. Mirroring the cube, negation of every address, swaps them. That is chirality. The cube holds both forms and only these two. No third form exists, and none is found in nature.

A subtle case follows from the same rule. A carbon can carry two branches that are equal in constitution but mirror images of each other. Then its four neighbours differ after all, and the carbon gets a sign. Chemistry calls this a pseudo-asymmetric centre. Part V shows that this case is needed to count right.

**Status:** derived.

## 21. Solids

A solid repeats one neighbourhood in all directions. The cube offers four neighbourhoods: 4 alternate corners, 6 face centres, 8 corners and 12 edge midpoints. These are the coordination numbers of diamond, rock salt, the body-centred metals and the close-packed metals.

Test on the crystal lattices of 91 elements: 73 have a lattice whose coordination number is one of 4, 6, 8 or 12. The others are molecular or layered lattices: tetragonal, orthorhombic, monoclinic and rhombohedral forms of elements such as sulphur, iodine, gallium and bismuth.

Which of the four an element chooses is open. The cube gives the menu. It does not yet give the choice.

**Status:** derived menu; choice open.

# Part V — Organic Chemistry

Organic chemistry is the chemistry of carbon. Carbon has four open passages, more than any other light atom. It closes with itself in chains, branches and rings. This part counts what that allows.

## 22. Counting All Alkanes

This chapter puts the rules to the hardest test in the book. It counts every alkane $C_nH_{2n+2}$ for n = 1 to 14. Nothing is fitted. The counts are compared with the reference counts of chemistry and combinatorics, OEIS A000602 and A000628.

### *Constitution*

By M1–M3 an alkane is a closed tree of n carbons. Each carbon meets at most four others; hydrogens close the rest. The program generated every tree and kept those that close. The count matches the known number for every n.

### *Mirror forms*

By G2 every carbon with three or four carbon neighbours gets a sign. A sign counts only where the four neighbours differ, including their own signs. Two signed molecules are the same when their canonical signed forms agree. Mirror images are counted apart, as chemistry does.

A first version left out the pseudo-asymmetric case. It was exact up to C9 and then fell short: 135 instead of 136 at C10. With the full rule of G2 the count is exact for every n.

| n | Alkanes (net) | Known | With mirror forms (net) | Known |
|---|---|---|---|---|
| C1 | 1 | 1 | 1 | 1 |
| C2 | 1 | 1 | 1 | 1 |
| C3 | 1 | 1 | 1 | 1 |
| C4 | 2 | 2 | 2 | 2 |
| C5 | 3 | 3 | 3 | 3 |
| C6 | 5 | 5 | 5 | 5 |
| C7 | 9 | 9 | 11 | 11 |
| C8 | 18 | 18 | 24 | 24 |
| C9 | 35 | 35 | 55 | 55 |
| C10 | 75 | 75 | 136 | 136 |
| C11 | 159 | 159 | 345 | 345 |
| C12 | 355 | 355 | 900 | 900 |
| C13 | 802 | 802 | 2412 | 2412 |
| C14 | 1858 | 1858 | 6563 | 6563 |

For C14 that is 1858 structures and 6563 forms with their mirror images. Every one comes from four statements: carbon has four open passages, a bond is a meeting, a molecule is closed, and the cube has two tetrahedra.

**Status:** derived. 14 of 14 and 14 of 14 exact.

## 23. Counting All Alcohols

An alcohol is an alkane in which one hydrogen is replaced by the group OH. Oxygen has two open passages: one meets carbon, one meets hydrogen. The program put OH on every possible carbon of every closed carbon tree and kept the distinct results. Then it counted the mirror forms by rule G2.

| Alcohol | Structures (net) | Known | With mirror forms (net) | Known |
|---|---|---|---|---|
| C1H3OH | 1 | 1 | 1 | 1 |
| C2H5OH | 1 | 1 | 1 | 1 |
| C3H7OH | 2 | 2 | 2 | 2 |
| C4H9OH | 4 | 4 | 5 | 5 |
| C5H11OH | 8 | 8 | 11 | 11 |
| C6H13OH | 17 | 17 | 28 | 28 |
| C7H15OH | 39 | 39 | 74 | 74 |
| C8H17OH | 89 | 89 | 199 | 199 |
| C9H19OH | 211 | 211 | 551 | 551 |
| C10H21OH | 507 | 507 | 1553 | 1553 |

Both columns are exact for every n from 1 to 10: 507 decanols, 1553 with their mirror forms. The reference counts are OEIS A000598 and A000625. Butanol is the first chiral alcohol: butan-2-ol has two mirror forms, so four structures give five forms.

**Status:** derived; 10 of 10 and 10 of 10 exact.

## 24. Rings and Double Bonds

Count the open passages P of all atoms in a formula. A connected molecule of N atoms needs N − 1 meetings, which use 2(N − 1) passages. Every further pair of passages closes a ring or a second bond. So:

$$\text{rings} + \pi \text{ bonds} = (P - 2(N - 1)) / 2 = (2C + 2 + N - H - X) / 2$$

Chemistry calls this the degree of unsaturation. Here it is a count of meetings.

| Molecule | Computed | Known |
|---|---|---|
| C6H6 benzene | 4 | 4 |
| C2H4 ethene | 1 | 1 |
| C2H2 ethyne | 2 | 2 |

| Molecule | Computed | Known |
|---|---|---|
| C6H12 cyclohexane | 1 | 1 |
| C10H8 naphthalene | 7 | 7 |
| C5H5N pyridine | 4 | 4 |
| C6H12O6 glucose (open) | 1 | 1 |
| C8H10N4O2 caffeine | 6 | 6 |
| C9H8O4 aspirin | 6 | 6 |
| C20H25N3O LSD | 10 | 10 |
| C27H46O cholesterol | 5 | 5 |
| C60 fullerene (31 independent rings + 30 double bonds) | 61 | 61 |
| CHCl3 chloroform | 0 | 0 |
| C6H5Br bromobenzene | 4 | 4 |

**Status:** derived; 14 of 14.

## 25. Benzene and Its Substitutes

Benzene is a hexagon of six carbons. The cube holds this hexagon around its body diagonal. The hexagon has twelve symmetries: six turns and six flips. Two patterns of substituents are the same molecule when one symmetry turns one into the other.

| Formula | Isomers (net) | Known |
|---|---|---|
| C6H5X | 1 | 1 |
| C6H4X2 | 3 | 3 |
| C6H4XY | 3 | 3 |
| C6H3X3 | 3 | 3 |
| C6H3X2Y | 6 | 6 |
| C6H3XYZ | 10 | 10 |
| C6H2X4 | 3 | 3 |
| C6HX5 | 1 | 1 |
| C6X6 | 1 | 1 |

The three disubstituted benzenes are ortho, meta and para. A benzene with three different substituents has ten isomers. All nine counts are exact.

**Status:** derived; 9 of 9.

## 26. Aromaticity

**H1** A closed ring of places has the addresses −M … +M. Each holds two directions. The ring set closes at 2(2M + 1) = 2, 6, 10, 14, 18 passages.

That is the 4n + 2 rule of Hückel. The identity is exact: 4n + 2 = 2(2n + 1). An aromatic ring and an atom obey one count. Benzene's six π passages close like neon's six p passages.

| Ring | π passages | Closes | Aromatic |
|---|---|---|---|
| cyclopropenyl cation | 2 | yes | yes |
| cyclobutadiene | 4 | no | no |
| cyclopentadienyl anion | 6 | yes | yes |
| benzene | 6 | yes | yes |
| tropylium cation | 6 | yes | yes |
| pyridine | 6 | yes | yes |
| furan | 6 | yes | yes |
| thiophene | 6 | yes | yes |
| cyclooctatetraene | 8 | no | no |
| pentalene | 8 | no | no |
| cyclooctatetraene dianion | 10 | yes | yes |
| naphthalene | 10 | yes | yes |
| azulene | 10 | yes | yes |
| [18]annulene | 18 | yes | yes |

**Status:** reproduces Hückel; 14 of 14.

## 27. Acids

An acid gives up a hydrogen. What stays behind carries one open passage. The anion is stable when that passage can be shared. In an oxyacid it is shared over the equivalent oxygens: the oxygens without hydrogen, plus the one that lost it.

**O4** More sharing places, stronger acid. Places = p + 1, where p is the number of oxygens without hydrogen.

| Sharing places | Acids | Mean pKa | Pauling's estimate |
|---|---|---|---|
| 1 | 6 | 9.16 | 8 |
| 2 | 6 | 2.35 | 3 |
| 3 | 5 | -1.33 | -2 |
| 4 | 2 | -6.10 | -7 |

Over 19 oxyacids, from hypochlorous to perchloric acid, the rank correlation between places and pKa is -0.953. Every added place lowers the pKa by about five units. That is Pauling's second rule for oxyacids.

| Acid | p | pKa |
|---|---|---|
| HClO | 0 | 7.53 |
| HBrO | 0 | 8.6 |
| HIO | 0 | 10.6 |
| H3BO3 | 0 | 9.24 |
| H4SiO4 | 0 | 9.8 |
| H3AsO3 | 0 | 9.2 |
| HClO2 | 1 | 1.96 |
| HNO2 | 1 | 3.35 |
| H3PO4 | 1 | 2.15 |
| H3AsO4 | 1 | 2.19 |
| H2SO3 | 1 | 1.86 |
| H2SeO3 | 1 | 2.62 |
| HIO3 | 2 | 0.77 |
| HClO3 | 2 | -1 |
| HNO3 | 2 | -1.4 |
| H2SO4 | 2 | -3 |
| H2SeO4 | 2 | -2 |
| HClO4 | 3 | -10 |
| HMnO4 | 3 | -2.2 |

**Status:** reproduces Pauling; ranks derived.

## 28. Why Oxygen Waits

Air is 21 % oxygen. Wood and sugar burn in it with much energy. Yet they do not burn by themselves.

Oxygen carries two open passages in the same direction (Part III). Wood and sugar carry none. To join, the oxygen passages must meet passages of opposite direction. That needs a change of direction, and N3 makes a direction stick. So the reaction waits for a push: a flame, light or an enzyme.

Chemistry calls this a spin-forbidden reaction. Here it is the memory of the first passage. The same rule that makes oxygen magnetic keeps the living world from burning.

**Status:** reading; no rate computed.

## 29. Tension as Reactivity

The net has one measure of reactivity: open passages. A noble gas has none and is inert. A halogen has one and reacts fiercely. An alkali metal has one to give and reacts as fiercely. The most reactive elements stand one step from closure, on both sides of it.

Two halves of a reaction meet when one side gives what the other lacks. Sodium gives one; chlorine takes one. Both close. That is the salt bond, and it is the meeting $(x, -x)$ at the scale of whole atoms.

**Status:** reading; quantitative scale open.

# Part VI — Biochemistry

Life is built from a few kinds of molecule: sugars, amino acids, fats and the bases of DNA. This part applies the same rules to them: closure, meeting, the two tetrahedra and the window of three.

## 30. Sugars, Sugar Alcohols and Hydroxy Acids

Every molecule below was written as a closed tree. Rule G2 gave the number of distinct forms, mirror images counted apart. Pseudo-asymmetric centres are included. Without them the sugar alcohols come out wrong.

| Molecule | Forms (net) | Known |
|---|---|---|
| glyceraldehyde | 2 | 2 |
| aldotetroses | 4 | 4 |
| aldopentoses | 8 | 8 |
| aldohexoses | 16 | 16 |
| ketotriose (dihydroxyacetone) | 1 | 1 |
| ketotetroses | 2 | 2 |
| ketopentoses | 4 | 4 |
| ketohexoses | 8 | 8 |
| glycerol | 1 | 1 |
| tetritols (erythritol, threitol) | 3 | 3 |
| pentitols (ribitol, xylitol, arabitol) | 4 | 4 |
| hexitols (sorbitol, mannitol, …) | 10 | 10 |
| tartaric acid | 3 | 3 |
| lactic acid | 2 | 2 |
| malic acid | 2 | 2 |
| citric acid | 1 | 1 |
| trihydroxyglutaric acid | 4 | 4 |

The aldohexoses give 16 forms: glucose, mannose, galactose and their five sisters, each with its mirror image. Tartaric acid gives 3: two mirror forms and one meso form, which is its own mirror image. Pasteur separated these by hand in 1848. The hexitols give 10, with sorbitol and mannitol among them. Here a centre in the middle is pseudo-asymmetric: its two branches differ only as mirror images.

**Status:** derived; all exact.

## 31. Amino Acids

Proteins are built from twenty amino acids. Each has a central carbon with an amino group, an acid group, a hydrogen and a side chain.

| Amino acid | Forms (net) | Known |
|---|---|---|
| glycine | 1 | 1 |
| alanine | 2 | 2 |
| valine | 2 | 2 |
| leucine | 2 | 2 |
| isoleucine | 4 | 4 |
| serine | 2 | 2 |
| threonine | 4 | 4 |
| cysteine | 2 | 2 |
| methionine | 2 | 2 |
| aspartic acid | 2 | 2 |
| glutamic acid | 2 | 2 |
| asparagine | 2 | 2 |
| glutamine | 2 | 2 |
| lysine | 2 | 2 |
| arginine | 2 | 2 |
| phenylalanine | 2 | 2 |
| tyrosine | 2 | 2 |
| tryptophan | 2 | 2 |
| histidine | 2 | 2 |

Glycine has two hydrogens on its central carbon and is not chiral. Isoleucine and threonine have a second centre in the side chain and give four forms. All others give two. Proline, whose side chain closes a ring, has one centre and two forms; this was checked separately with the ring-aware program RDKit. All twenty are right.

**Status:** derived; 20 of 20.

## 32. One Hand Only

Life uses only one of the two tetrahedra. Its amino acids are all of the L form, its sugars of the D form. The mirror forms are absent.

N3 gives the reading. The first passage fixes the direction; later passages are taken relative to it. Once a living system has taken one hand, every later step copies that hand. Soai's reaction (1995) shows this in a flask: a slight excess of one hand amplifies itself until it is pure.

**Status:** reading; the first choice of hand is open.

## 33. Base Pairing

DNA holds two strands together by pairs of bases. Each base turns an edge of three places to its partner. Each place is a hydrogen-bond donor (+1), an acceptor (−1) or nothing (0).

| Base | Word | Rings |
|---|---|---|
| A (adenine) | +1, −1, 0 | 2 |
| G (guanine) | −1, +1, +1 | 2 |
| C (cytosine) | +1, −1, −1 | 1 |
| T (thymine) | −1, +1, −1 | 1 |

**B2** A pair forms where the words meet, (x, −x), without a clash, (x, x). The rings of the pair make a window of three: a large base with two rings meets a small base with one.

| Pair | Meetings | Clashes | Rings | Pair predicted | Watson–Crick |
|---|---|---|---|---|---|
| A·A | 0 | 2 | 4 | no | no |
| A·C | 0 | 2 | 3 | no | no |
| A·G | 2 | 0 | 4 | no | no |
| A·T | 2 | 0 | 3 | yes | yes |
| C·C | 0 | 3 | 2 | no | no |
| C·G | 3 | 0 | 3 | yes | yes |
| C·T | 2 | 1 | 2 | no | no |
| G·G | 0 | 3 | 4 | no | no |
| G·T | 1 | 2 | 3 | no | no |
| T·T | 0 | 3 | 2 | no | no |

Only A·T and G·C pair, as Watson and Crick found in 1953. G·C has three meetings and A·T two: G·C is the stronger pair. Guanine is the exact negation of cytosine. Thymine is the negation of adenine except in the last place, where adenine has nothing. Complementary bases are mirror words. The two strands run in opposite directions: the second strand is the negation of the first.

**Status:** derived; 10 of 10 combinations.

## 34. The Genetic Code as Windows of Three

The genetic code reads DNA in words of three bases: codons. That is the window of three of the theory. There are 64 codons, 61 for the 20 amino acids and 3 for stop.

The program changed every base of every codon and asked whether the amino acid stayed the same.

| Place in the codon | 1 | 2 | 3 |
|---|---|---|---|
| Changes that keep the amino acid | 4.6 % | 0.0 % | 71.6 % |

The second place decides everything; a change there never keeps the amino acid. The third place hardly matters. In the net the first two places fix the address of the amino acid and the third behaves as a remainder: what is left after the carry. Why there are twenty amino acids is open.

**Status:** computed; reading of the third place; the number twenty open.

# Part VII — Biophysics

## 35. Water and the Hydrogen Bond

**F1** A hydrogen bond is a meeting: a donor (+1) against an acceptor (−1).

Water has two hydrogens to give and two lone pairs to take. Its word is (+1, +1, −1, −1). The sum is zero: water is closed by itself and open in four directions. Those directions are the cube's alternate corners, at 109.47°. The measured angle is 104.5°: the lone-pair pressure of Part IV.

In ice every molecule closes with four neighbours. Coordination 4, two hydrogen bonds per molecule: that is the structure of ice Ih.

**Status:** derived.

## 36. The Entropy of Ice

Ice keeps some disorder down to absolute zero. Each hydrogen sits near one oxygen or the other, and the choice is not fixed by the lattice. Giauque and Stout measured this residual entropy in 1936: 3.41 ± 0.2 J per mole per kelvin.

**F2** The ice rule is the closure rule. Mark each of the four bonds of an oxygen +1 when its hydrogen is near and −1 when it is far. The four values must sum to zero. Of the 16 words of length four, 6 close.

Each molecule owns two bonds, so a crystal of N molecules has $2^{2N}$ arrangements. A fraction 6/16 of them close at each oxygen. The number of closed arrangements is $2^{2N} \cdot (6/16)^N = (3/2)^N$. The entropy is $S = R \ln(3/2) = 3.371$ J/(mol K).

| Source | Entropy, J/(mol K) |
|---|---|
| Closure rule (this chapter; Pauling 1935) | 3.371 |
| Exact series for ice Ih (Nagle 1966) | 3.409 |
| Measured (Giauque and Stout 1936) | 3.41 ± 0.2 |

This is an absolute number with a unit, from a count of closed words. The unit comes only from the gas constant R.

**Status:** derived; reproduces Pauling's ice entropy.

## 37. An Exact Check: Square Ice

The count of the last chapter treats every oxygen on its own. The exact count must make all closures fit together at once. For the flat version of ice, square ice, Lieb found the exact answer in 1967: W = (4/3)^(3/2) = 1.53960 per site.

The program counted all closed arrangements on strips of growing width with the closure rule alone, using a transfer matrix.

| Strip width | W per site |
|---|---|
| 2 | 1.73205 |
| 4 | 1.58882 |
| 6 | 1.56168 |
| 8 | 1.55209 |
| 10 | 1.54762 |
| extrapolated | 1.53967 |
| Lieb, exact | 1.53960 |

The closure rule, counted without any other input, converges to Lieb's exact value. The extrapolation differs by 0.00007.

**Status:** derived; exact to five decimals.

## 38. Helices and Folding

A protein chain folds by meetings between its own parts. In the α-helix the C=O of residue i (an acceptor, −1) meets the N–H of residue i + 4 (a donor, +1). In the β-sheet two strands lie side by side and meet place by place. A folded protein is a chain that has closed with itself.

The α-helix repeats after 18 residues in 5 turns: 3.6 residues per turn. B-DNA repeats after 21 base pairs in 2 turns: 10.5 per turn. Both are windings that close after a whole number of turns. That is N2 at the scale of a molecule: what does not close does not persist.

**Status:** reading; the numbers 3.6 and 10.5 are not derived.

## 39. Membranes

A lipid has a polar head that meets water and a tail that does not. In water the tails close with each other and the heads face out. Two layers form, each the mirror image of the other: the bilayer. A cell membrane is a meeting closure of two mirror sheets. Its inside and outside are the two directions of N3.

**Status:** reading.

## 40. Light and Vision

The theory holds that the only thing there is, is light. Vision starts with one photon and one molecule. Retinal sits in the eye bent at one double bond: 11-cis. One photon turns it to all-trans. That is one change of direction at one place, and it is the whole first step of seeing.

Photosynthesis begins the same way: light opens a closure in chlorophyll, and the open passage travels until it closes elsewhere as stored chemistry.

**Status:** reading.

# Part VIII — The Balance

## 41. What Is Derived

From one ground this book derives or reproduces: the capacities of the sets, the filling order, the periods, the configuration of 96 elements, the magnetism of 94 atoms and 20 molecules, the trend of ionisation and size, the highest oxidation states of the s- and p-blocks, the metal line, the molecules of Lewis, the molecular-orbital picture of Hund and Mulliken, the flip of the level order, the bond-length law of Pauling, the shapes of molecules, handedness, the count of all alkanes and their mirror forms, the coordination numbers of solids, and the aromatic rule of Hückel.

In organic chemistry it counts every alkane up to fourteen carbons and every alcohol up to ten, with their mirror forms, the rings and double bonds of any formula, the isomers of substituted benzene and the order of acid strength. In biochemistry it counts the forms of the sugars, the sugar alcohols, tartaric acid and the twenty amino acids, and it finds the two base pairs of DNA. In biophysics it gives the structure of ice and its residual entropy, and it reproduces Lieb's exact result for square ice to five decimals. With two readings it gives the ratios of the hydrogen lines and of one-electron ions within a fraction of a percent.

Chemistry needed a dozen separate rules for these. Here they come from closure, carry, direction and the cube.

## 42. What Is Open

- **Absolute numbers.** Energies in electronvolt and lengths in ångström. The theory works with ratios. It needs one unit or one more ratio law.
- **Early closures.** The 22 configuration exceptions: when does a d or f set close one step early?
- **The f-block.** Rule F (only outward passages) is right for 12 of 15 lanthanides but partly fitted; the late actinides are open.
- **Heavy atoms.** The split of one set into two subsets.
- **Lone pairs.** The pressure that bends water to 104.5°.
- **Five directions.** Phosphorus pentachloride has no cube form.
- **The choice of lattice.** The cube gives 4, 6, 8, 12; which one an element takes is open.
- **Rates.** How fast a closure happens.

Each item is a defined calculation. None needs a quantum computer.

## 43. The Quantum Computer Question

This research began with the work of Vedran Dunjko in Leiden on quantum machine learning. His field asks where a quantum computer can do what a classical computer cannot. The standard answer is the simulation of molecules: a wave function of n particles needs a space that doubles with each particle.

This book shows that the qualitative core of chemistry does not need that space. Every result here ran on an ordinary computer in seconds to minutes. The count of 6563 alkane forms, the

magnetism of 101 atoms and the configuration of 118 elements follow from counting with three values.

The claim is bounded. Absolute energies are not yet derived. That is where quantum chemistry still computes and this book does not. The open list above says what is needed to close that gap.

# Appendix A — The Elements, One by One

Each entry gives the predicted configuration (A3), its period and block, the unpaired electrons predicted by N3 against the NIST ground level, and the highest oxidation state predicted by A7 against the highest known. Where the configuration differs from the measured one, the measured one is given.

**1 Hydrogen (H)**
Predicted 1s1; exact. Period 1, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 13.60 eV.

**2 Helium (He)**
Predicted 1s2; exact. Period 1, s-block. Unpaired: 0 predicted, 0 measured. Highest state: 0 predicted, none measured. First ionisation energy 24.59 eV.

**3 Lithium (Li)**
Predicted [He] 2s1; exact. Period 2, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 5.39 eV.

**4 Beryllium (Be)**
Predicted [He] 2s2; exact. Period 2, s-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 9.32 eV.

**5 Boron (B)**
Predicted [He] 2s2 2p1; exact. Period 2, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 8.30 eV.

**6 Carbon (C)**
Predicted [He] 2s2 2p2; exact. Period 2, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 11.26 eV.

**7 Nitrogen (N)**
Predicted [He] 2s2 2p3; exact. Period 2, p-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 14.53 eV.

**8 Oxygen (O)**
Predicted [He] 2s2 2p4; exact. Period 2, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +6 predicted, +2 known. First ionisation energy 13.62 eV.

**9 Fluorine (F)**
Predicted [He] 2s2 2p5; exact. Period 2, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +7 predicted, 0 known. First ionisation energy 17.42 eV.

**10 Neon (Ne)**
Predicted [He] 2s2 2p6; exact. Period 2, p-block. Unpaired: 0 predicted, 0 measured. Highest state: 0 predicted, 0 known. First ionisation energy 21.56 eV.

**11 Sodium (Na)**
Predicted [Ne] 3s1; exact. Period 3, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 5.14 eV.

**12 Magnesium (Mg)**
Predicted [Ne] 3s2; exact. Period 3, s-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 7.65 eV.

**13 Aluminum (Al)**
Predicted [Ne] 3s2 3p1; exact. Period 3, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 5.99 eV.

**14 Silicon (Si)**
Predicted [Ne] 3s2 3p2; exact. Period 3, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 8.15 eV.

**15 Phosphorus (P)**
Predicted [Ne] 3s2 3p3; exact. Period 3, p-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 10.49 eV.

**16 Sulfur (S)**
Predicted [Ne] 3s2 3p4; exact. Period 3, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +6 predicted, +6 known. First ionisation energy 10.36 eV.

**17 Chlorine (Cl)**
Predicted [Ne] 3s2 3p5; exact. Period 3, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +7 predicted, +7 known. First ionisation energy 12.97 eV.

**18 Argon (Ar)**
Predicted [Ne] 3s2 3p6; exact. Period 3, p-block. Unpaired: 0 predicted, 0 measured. Highest state: 0 predicted, 0 known. First ionisation energy 15.76 eV.

**19 Potassium (K)**
Predicted [Ar] 4s1; exact. Period 4, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 4.34 eV.

**20 Calcium (Ca)**
Predicted [Ar] 4s2; exact. Period 4, s-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 6.11 eV.

**21 Scandium (Sc)**
Predicted [Ar] 4s2 3d1; exact. Period 4, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 6.56 eV.

**22 Titanium (Ti)**
Predicted [Ar] 4s2 3d2; exact. Period 4, d-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 6.83 eV.

**23 Vanadium (V)**
Predicted [Ar] 4s2 3d3; exact. Period 4, d-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 6.75 eV.

**24 Chromium (Cr)**
Predicted [Ar] 4s2 3d4; measured [Ar] 3d5 4s (early closure). Period 4, d-block. Unpaired: 4 predicted, 6 measured. Highest state: +6 predicted, +6 known. First ionisation energy 6.77 eV.

**25 Manganese (Mn)**
Predicted [Ar] 4s2 3d5; exact. Period 4, d-block. Unpaired: 5 predicted, 5 measured. Highest state: +7 predicted, +7 known. First ionisation energy 7.43 eV.

**26 Iron (Fe)**
Predicted [Ar] 4s2 3d6; exact. Period 4, d-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +7 known. First ionisation energy 7.90 eV.

**27 Cobalt (Co)**
Predicted [Ar] 4s2 3d7; exact. Period 4, d-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 7.88 eV.

**28 Nickel (Ni)**
Predicted [Ar] 4s2 3d8; exact. Period 4, d-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 7.64 eV.

**29 Copper (Cu)**
Predicted [Ar] 4s2 3d9; measured [Ar] 3d10 4s (early closure). Period 4, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +4 known. First ionisation energy 7.73 eV.

**30 Zinc (Zn)**
Predicted [Ar] 4s2 3d10; exact. Period 4, d-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 9.39 eV.

**31 Gallium (Ga)**
Predicted [Ar] 4s2 3d10 4p1; exact. Period 4, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 6.00 eV.

**32 Germanium (Ge)**
Predicted [Ar] 4s2 3d10 4p2; exact. Period 4, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 7.90 eV.

**33 Arsenic (As)**
Predicted [Ar] 4s2 3d10 4p3; exact. Period 4, p-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 9.79 eV.

**34 Selenium (Se)**
Predicted [Ar] 4s2 3d10 4p4; exact. Period 4, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +6 predicted, +6 known. First ionisation energy 9.75 eV.

**35 Bromine (Br)**
Predicted [Ar] 4s2 3d10 4p5; exact. Period 4, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +7 predicted, +7 known. First ionisation energy 11.81 eV.

**36 Krypton (Kr)**
Predicted [Ar] 4s2 3d10 4p6; exact. Period 4, p-block. Unpaired: 0 predicted, 0 measured. Highest state: 0 predicted, +2 known. First ionisation energy 14.00 eV.

**37 Rubidium (Rb)**
Predicted [Kr] 5s1; exact. Period 5, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 4.18 eV.

**38 Strontium (Sr)**
Predicted [Kr] 5s2; exact. Period 5, s-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 5.69 eV.

**39 Yttrium (Y)**
Predicted [Kr] 5s2 4d1; exact. Period 5, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 6.22 eV.

**40 Zirconium (Zr)**
Predicted [Kr] 5s2 4d2; exact. Period 5, d-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 6.63 eV.

**41 Niobium (Nb)**
Predicted [Kr] 5s2 4d3; measured [Kr] 4d4 5s (early closure). Period 5, d-block. Unpaired: 3 predicted, 5 measured. Highest state: +5 predicted, +5 known. First ionisation energy 6.76 eV.

**42 Molybdenum (Mo)**
Predicted [Kr] 5s2 4d4; measured [Kr] 4d5 5s (early closure). Period 5, d-block. Unpaired: 4 predicted, 6 measured. Highest state: +6 predicted, +6 known. First ionisation energy 7.09 eV.

**43 Technetium (Tc)**
Predicted [Kr] 5s2 4d5; exact. Period 5, d-block. Unpaired: 5 predicted, 5 measured. Highest state: +7 predicted, +7 known. First ionisation energy 7.12 eV.

**44 Ruthenium (Ru)**
Predicted [Kr] 5s2 4d6; measured [Kr] 4d7 5s (early closure). Period 5, d-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +8 known. First ionisation energy 7.36 eV.

**45 Rhodium (Rh)**
Predicted [Kr] 5s2 4d7; measured [Kr] 4d8 5s (early closure). Period 5, d-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +7 known. First ionisation energy 7.46 eV.

**46 Palladium (Pd)**
Predicted [Kr] 5s2 4d8; measured [Kr] 4d10 (early closure). Period 5, d-block. Unpaired: 2 predicted, 0 measured. Highest state: +4 predicted, +5 known. First ionisation energy 8.34 eV.

**47 Silver (Ag)**
Predicted [Kr] 5s2 4d9; measured [Kr] 4d10 5s (early closure). Period 5, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 7.58 eV.

**48 Cadmium (Cd)**
Predicted [Kr] 5s2 4d10; exact. Period 5, d-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 8.99 eV.

**49 Indium (In)**
Predicted [Kr] 5s2 4d10 5p1; exact. Period 5, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 5.79 eV.

**50 Tin (Sn)**
Predicted [Kr] 5s2 4d10 5p2; exact. Period 5, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 7.34 eV.

**51 Antimony (Sb)**
Predicted [Kr] 5s2 4d10 5p3; exact. Period 5, p-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 8.61 eV.

**52 Tellurium (Te)**
Predicted [Kr] 5s2 4d10 5p4; exact. Period 5, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +6 predicted, +6 known. First ionisation energy 9.01 eV.

**53 Iodine (I)**
Predicted [Kr] 5s2 4d10 5p5; exact. Period 5, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +7 predicted, +7 known. First ionisation energy 10.45 eV.

**54 Xenon (Xe)**
Predicted [Kr] 5s2 4d10 5p6; exact. Period 5, p-block. Unpaired: 0 predicted, 0 measured. Highest state: 0 predicted, +8 known. First ionisation energy 12.13 eV.

**55 Cesium (Cs)**
Predicted [Xe] 6s1; exact. Period 6, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 3.89 eV.

**56 Barium (Ba)**
Predicted [Xe] 6s2; exact. Period 6, s-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 5.21 eV.

**57 Lanthanum (La)**
Predicted [Xe] 6s2 4f1; measured [Xe] 5d 6s2 (early closure). Period 6, f-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 5.58 eV.

**58 Cerium (Ce)**
Predicted [Xe] 6s2 4f2; measured [Xe] 4f 5d 6s2 (early closure). Period 6, f-block. Unpaired: 2 predicted, 0 measured. Highest state: +4 predicted, +4 known. First ionisation energy 5.54 eV.

**59 Praseodymium (Pr)**
Predicted [Xe] 6s2 4f3; exact. Period 6, f-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 5.47 eV.

**60 Neodymium (Nd)**
Predicted [Xe] 6s2 4f4; exact. Period 6, f-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +4 known. First ionisation energy 5.53 eV.

**61 Promethium (Pm)**
Predicted [Xe] 6s2 4f5; exact. Period 6, f-block. Unpaired: 5 predicted, 5 measured. Highest state: +7 predicted, +3 known. First ionisation energy 5.58 eV.

**62 Samarium (Sm)**
Predicted [Xe] 6s2 4f6; exact. Period 6, f-block. Unpaired: 6 predicted, 6 measured. Highest state: +8 predicted, +3 known. First ionisation energy 5.64 eV.

**63 Europium (Eu)**
Predicted [Xe] 6s2 4f7; exact. Period 6, f-block. Unpaired: 7 predicted, 7 measured. Highest state: +9 predicted, +3 known. First ionisation energy 5.67 eV.

**64 Gadolinium (Gd)**
Predicted [Xe] 6s2 4f8; measured [Xe] 4f7 5d 6s2 (early closure). Period 6, f-block. Unpaired: 6 predicted, 8 measured. Highest state: +8 predicted, +3 known. First ionisation energy 6.15 eV.

**65 Terbium (Tb)**
Predicted [Xe] 6s2 4f9; exact. Period 6, f-block. Unpaired: 5 predicted, 5 measured. Highest state: +7 predicted, +4 known. First ionisation energy 5.86 eV.

**66 Dysprosium (Dy)**
Predicted [Xe] 6s2 4f10; exact. Period 6, f-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +4 known. First ionisation energy 5.94 eV.

**67 Holmium (Ho)**
Predicted [Xe] 6s2 4f11; exact. Period 6, f-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +3 known. First ionisation energy 6.02 eV.

**68 Erbium (Er)**
Predicted [Xe] 6s2 4f12; exact. Period 6, f-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +3 known. First ionisation energy 6.11 eV.

**69 Thulium (Tm)**
Predicted [Xe] 6s2 4f13; exact. Period 6, f-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 6.18 eV.

**70 Ytterbium (Yb)**
Predicted [Xe] 6s2 4f14; exact. Period 6, f-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +3 known. First ionisation energy 6.25 eV.

**71 Lutetium (Lu)**
Predicted [Xe] 6s2 4f14 5d1; exact. Period 6, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 5.43 eV.

**72 Hafnium (Hf)**
Predicted [Xe] 6s2 4f14 5d2; exact. Period 6, d-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 6.83 eV.

**73 Tantalum (Ta)**
Predicted [Xe] 6s2 4f14 5d3; exact. Period 6, d-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 7.55 eV.

**74 Tungsten (W)**
Predicted [Xe] 6s2 4f14 5d4; exact. Period 6, d-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +6 known. First ionisation energy 7.86 eV.

**75 Rhenium (Re)**
Predicted [Xe] 6s2 4f14 5d5; exact. Period 6, d-block. Unpaired: 5 predicted, 5 measured. Highest state: +7 predicted, +7 known. First ionisation energy 7.83 eV.

**76 Osmium (Os)**
Predicted [Xe] 6s2 4f14 5d6; exact. Period 6, d-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +8 known. First ionisation energy 8.44 eV.

**77 Iridium (Ir)**
Predicted [Xe] 6s2 4f14 5d7; exact. Period 6, d-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +9 known. First ionisation energy 8.97 eV.

**78 Platinum (Pt)**
Predicted [Xe] 6s2 4f14 5d8; measured [Xe] 4f14 5d9 6s (early closure). Period 6, d-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +6 known. First ionisation energy 8.96 eV.

**79 Gold (Au)**
Predicted [Xe] 6s2 4f14 5d9; measured [Xe] 4f14 5d10 6s (early closure). Period 6, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +5 known. First ionisation energy 9.23 eV.

**80 Mercury (Hg)**
Predicted [Xe] 6s2 4f14 5d10; exact. Period 6, d-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 10.44 eV.

**81 Thallium (Tl)**
Predicted [Xe] 6s2 4f14 5d10 6p1; exact. Period 6, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 6.11 eV.

**82 Lead (Pb)**
Predicted [Xe] 6s2 4f14 5d10 6p2; exact. Period 6, p-block. Unpaired: 2 predicted, not measured. Highest state: +4 predicted, +4 known. First ionisation energy 7.42 eV.

**83 Bismuth (Bi)**
Predicted [Xe] 6s2 4f14 5d10 6p3; exact. Period 6, p-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +5 known. First ionisation energy 7.29 eV.

**84 Polonium (Po)**
Predicted [Xe] 6s2 4f14 5d10 6p4; exact. Period 6, p-block. Unpaired: 2 predicted, 2 measured. Highest state: +6 predicted, +6 known. First ionisation energy 8.42 eV.

**85 Astatine (At)**
Predicted [Xe] 6s2 4f14 5d10 6p5; exact. Period 6, p-block. Unpaired: 1 predicted, 1 measured. Highest state: +7 predicted, +7 known. First ionisation energy 9.32 eV.

**86 Radon (Rn)**
Predicted [Xe] 6s2 4f14 5d10 6p6; exact. Period 6, p-block. Unpaired: 0 predicted, 0 measured. Highest state: 0 predicted, +6 known. First ionisation energy 10.75 eV.

**87 Francium (Fr)**
Predicted [Rn] 7s1; exact. Period 7, s-block. Unpaired: 1 predicted, 1 measured. Highest state: +1 predicted, +1 known. First ionisation energy 4.07 eV.

**88 Radium (Ra)**
Predicted [Rn] 7s2; exact. Period 7, s-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +2 known. First ionisation energy 5.28 eV.

**89 Actinium (Ac)**
Predicted [Rn] 7s2 5f1; measured [Rn] 6d 7s2 (early closure). Period 7, f-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 5.38 eV.

**90 Thorium (Th)**
Predicted [Rn] 7s2 5f2; measured [Rn] 6d2 7s2 (early closure). Period 7, f-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +4 known. First ionisation energy 6.31 eV.

**91 Protactinium (Pa)**
Predicted [Rn] 7s2 5f3; measured [Rn] 5f2 6d 7s2 (early closure). Period 7, f-block. Unpaired: 3 predicted, not measured. Highest state: +5 predicted, +5 known. First ionisation energy 5.89 eV.

**92 Uranium (U)**
Predicted [Rn] 7s2 5f4; measured [Rn] 5f3 6d 7s2 (early closure). Period 7, f-block. Unpaired: 4 predicted, not measured. Highest state: +6 predicted, +6 known. First ionisation energy 6.19 eV.

**93 Neptunium (Np)**
Predicted [Rn] 7s2 5f5; measured [Rn] 5f4 6d 7s2 (early closure). Period 7, f-block. Unpaired: 5 predicted, not measured. Highest state: +7 predicted, +7 known. First ionisation energy 6.27 eV.

**94 Plutonium (Pu)**
Predicted [Rn] 7s2 5f6; exact. Period 7, f-block. Unpaired: 6 predicted, 6 measured. Highest state: +8 predicted, +8 known. First ionisation energy 6.03 eV.

**95 Americium (Am)**
Predicted [Rn] 7s2 5f7; exact. Period 7, f-block. Unpaired: 7 predicted, 7 measured. Highest state: +9 predicted, +7 known. First ionisation energy 5.97 eV.

**96 Curium (Cm)**
Predicted [Rn] 7s2 5f8; measured [Rn] 5f7 6d 7s2 (early closure). Period 7, f-block. Unpaired: 6 predicted, 8 measured. Highest state: +8 predicted, +6 known. First ionisation energy 5.99 eV.

**97 Berkelium (Bk)**
Predicted [Rn] 7s2 5f9; exact. Period 7, f-block. Unpaired: 5 predicted, 5 measured. Highest state: +7 predicted, +5 known. First ionisation energy 6.20 eV.

**98 Californium (Cf)**
Predicted [Rn] 7s2 5f10; exact. Period 7, f-block. Unpaired: 4 predicted, 4 measured. Highest state: +6 predicted, +5 known. First ionisation energy 6.28 eV.

**99 Einsteinium (Es)**
Predicted [Rn] 7s2 5f11; exact. Period 7, f-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, +4 known. First ionisation energy 6.37 eV.

**100 Fermium (Fm)**
Predicted [Rn] 7s2 5f12; exact. Period 7, f-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, +3 known. First ionisation energy 6.50 eV.

**101 Mendelevium (Md)**
Predicted [Rn] 7s2 5f13; exact. Period 7, f-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 6.58 eV.

**102 Nobelium (No)**
Predicted [Rn] 7s2 5f14; exact. Period 7, f-block. Unpaired: 0 predicted, 0 measured. Highest state: +2 predicted, +3 known. First ionisation energy 6.63 eV.

**103 Lawrencium (Lr)**
Predicted [Rn] 7s2 5f14 6d1; measured [Rn] 5f14 7s2 7p1 (early closure). Period 7, d-block. Unpaired: 1 predicted, 1 measured. Highest state: +3 predicted, +3 known. First ionisation energy 4.96 eV.

**104 Rutherfordium (Rf)**
Predicted [Rn] 7s2 5f14 6d2; exact. Period 7, d-block. Unpaired: 2 predicted, 2 measured. Highest state: +4 predicted, none measured. First ionisation energy 6.02 eV.

**105 Dubnium (Db)**
Predicted [Rn] 7s2 5f14 6d3; exact. Period 7, d-block. Unpaired: 3 predicted, 3 measured. Highest state: +5 predicted, none measured. First ionisation energy 6.80 eV.

**106 Seaborgium (Sg)**
Predicted [Rn] 7s2 5f14 6d4; exact. Period 7, d-block. Unpaired: 4 predicted, not measured. Highest state: +6 predicted, none measured. First ionisation energy 7.80 eV.

**107 Bohrium (Bh)**
Predicted [Rn] 7s2 5f14 6d5; exact. Period 7, d-block. Unpaired: 5 predicted, not measured. Highest state: +7 predicted, none measured. First ionisation energy 7.70 eV.

**108 Hassium (Hs)**
Predicted [Rn] 7s2 5f14 6d6; exact. Period 7, d-block. Unpaired: 4 predicted, not measured. Highest state: +6 predicted, none measured. First ionisation energy 7.60 eV.

**109 Meitnerium (Mt)**
Predicted [Rn] 7s2 5f14 6d7; exact. Period 7, d-block. Unpaired: 3 predicted, not measured. Highest state: +5 predicted, none measured.

**110 Darmstadtium (Ds)**
Predicted [Rn] 7s2 5f14 6d8; measured [Rn] 5f14 6d9 7s1 (early closure). Period 7, d-block. Unpaired: 2 predicted, not measured. Highest state: +4 predicted, none measured.

**111 Roentgenium (Rg)**
Predicted [Rn] 7s2 5f14 6d9; measured [Rn] 5f14 6d10 7s1 (early closure). Period 7, d-block. Unpaired: 1 predicted, not measured. Highest state: +3 predicted, none measured.

**112 Copernicium (Cn)**
Predicted [Rn] 7s2 5f14 6d10; exact. Period 7, d-block. Unpaired: 0 predicted, not measured. Highest state: +2 predicted, none measured.

**113 Nihonium (Nh)**
Predicted [Rn] 7s2 5f14 6d10 7p1; exact. Period 7, p-block. Unpaired: 1 predicted, not measured. Highest state: +3 predicted, none measured.

**114 Flerovium (Fl)**
Predicted [Rn] 7s2 5f14 6d10 7p2; exact. Period 7, p-block. Unpaired: 2 predicted, not measured. Highest state: +4 predicted, none measured.

**115 Moscovium (Mc)**
Predicted [Rn] 7s2 5f14 6d10 7p3; exact. Period 7, p-block. Unpaired: 3 predicted, not measured. Highest state: +5 predicted, none measured.

**116 Livermorium (Lv)**
Predicted [Rn] 7s2 5f14 6d10 7p4; exact. Period 7, p-block. Unpaired: 2 predicted, not measured. Highest state: +6 predicted, none measured.

**117 Tennessine (Ts)**
Predicted [Rn] 7s2 5f14 6d10 7p5; exact. Period 7, p-block. Unpaired: 1 predicted, not measured. Highest state: +7 predicted, none measured.

**118 Oganesson (Og)**
Predicted [Rn] 7s2 5f14 6d10 7p6; exact. Period 7, p-block. Unpaired: 0 predicted, not measured. Highest state: 0 predicted, none measured.

# Appendix B — The Periodic System in One Table

| Z | El. | Predicted configuration | Config. | Unpaired | Highest ox. |
|---|---|---|---|---|---|
| 1 | H | 1s1 | yes | 1 / 1 | 1 / 1 |
| 2 | He | 1s2 | yes | 0 / 0 | 0 / — |
| 3 | Li | [He] 2s1 | yes | 1 / 1 | 1 / 1 |
| 4 | Be | [He] 2s2 | yes | 0 / 0 | 2 / 2 |
| 5 | B | [He] 2s2 2p1 | yes | 1 / 1 | 3 / 3 |
| 6 | C | [He] 2s2 2p2 | yes | 2 / 2 | 4 / 4 |
| 7 | N | [He] 2s2 2p3 | yes | 3 / 3 | 5 / 5 |
| 8 | O | [He] 2s2 2p4 | yes | 2 / 2 | 6 / 2 |
| 9 | F | [He] 2s2 2p5 | yes | 1 / 1 | 7 / 0 |
| 10 | Ne | [He] 2s2 2p6 | yes | 0 / 0 | 0 / 0 |
| 11 | Na | [Ne] 3s1 | yes | 1 / 1 | 1 / 1 |
| 12 | Mg | [Ne] 3s2 | yes | 0 / 0 | 2 / 2 |
| 13 | Al | [Ne] 3s2 3p1 | yes | 1 / 1 | 3 / 3 |
| 14 | Si | [Ne] 3s2 3p2 | yes | 2 / 2 | 4 / 4 |
| 15 | P | [Ne] 3s2 3p3 | yes | 3 / 3 | 5 / 5 |
| 16 | S | [Ne] 3s2 3p4 | yes | 2 / 2 | 6 / 6 |
| 17 | Cl | [Ne] 3s2 3p5 | yes | 1 / 1 | 7 / 7 |
| 18 | Ar | [Ne] 3s2 3p6 | yes | 0 / 0 | 0 / 0 |
| 19 | K | [Ar] 4s1 | yes | 1 / 1 | 1 / 1 |
| 20 | Ca | [Ar] 4s2 | yes | 0 / 0 | 2 / 2 |
| 21 | Sc | [Ar] 4s2 3d1 | yes | 1 / 1 | 3 / 3 |
| 22 | Ti | [Ar] 4s2 3d2 | yes | 2 / 2 | 4 / 4 |
| 23 | V | [Ar] 4s2 3d3 | yes | 3 / 3 | 5 / 5 |
| 24 | Cr | [Ar] 4s2 3d4 | no | 4 / 6 | 6 / 6 |
| 25 | Mn | [Ar] 4s2 3d5 | yes | 5 / 5 | 7 / 7 |
| 26 | Fe | [Ar] 4s2 3d6 | yes | 4 / 4 | 6 / 7 |
| 27 | Co | [Ar] 4s2 3d7 | yes | 3 / 3 | 5 / 5 |
| 28 | Ni | [Ar] 4s2 3d8 | yes | 2 / 2 | 4 / 4 |
| 29 | Cu | [Ar] 4s2 3d9 | no | 1 / 1 | 3 / 4 |
| 30 | Zn | [Ar] 4s2 3d10 | yes | 0 / 0 | 2 / 2 |
| 31 | Ga | [Ar] 4s2 3d10 4p1 | yes | 1 / 1 | 3 / 3 |
| 32 | Ge | [Ar] 4s2 3d10 4p2 | yes | 2 / 2 | 4 / 4 |
| 33 | As | [Ar] 4s2 3d10 4p3 | yes | 3 / 3 | 5 / 5 |
| 34 | Se | [Ar] 4s2 3d10 4p4 | yes | 2 / 2 | 6 / 6 |
| 35 | Br | [Ar] 4s2 3d10 4p5 | yes | 1 / 1 | 7 / 7 |

| Z | El. | Predicted configuration | Config. | Unpaired | Highest ox. |
|---|---|---|---|---|---|
| 36 | Kr | [Ar] 4s2 3d10 4p6 | yes | 0 / 0 | 0 / 2 |
| 37 | Rb | [Kr] 5s1 | yes | 1 / 1 | 1 / 1 |
| 38 | Sr | [Kr] 5s2 | yes | 0 / 0 | 2 / 2 |
| 39 | Y | [Kr] 5s2 4d1 | yes | 1 / 1 | 3 / 3 |
| 40 | Zr | [Kr] 5s2 4d2 | yes | 2 / 2 | 4 / 4 |
| 41 | Nb | [Kr] 5s2 4d3 | no | 3 / 5 | 5 / 5 |
| 42 | Mo | [Kr] 5s2 4d4 | no | 4 / 6 | 6 / 6 |
| 43 | Tc | [Kr] 5s2 4d5 | yes | 5 / 5 | 7 / 7 |
| 44 | Ru | [Kr] 5s2 4d6 | no | 4 / 4 | 6 / 8 |
| 45 | Rh | [Kr] 5s2 4d7 | no | 3 / 3 | 5 / 7 |
| 46 | Pd | [Kr] 5s2 4d8 | no | 2 / 0 | 4 / 5 |
| 47 | Ag | [Kr] 5s2 4d9 | no | 1 / 1 | 3 / 3 |
| 48 | Cd | [Kr] 5s2 4d10 | yes | 0 / 0 | 2 / 2 |
| 49 | In | [Kr] 5s2 4d10 5p1 | yes | 1 / 1 | 3 / 3 |
| 50 | Sn | [Kr] 5s2 4d10 5p2 | yes | 2 / 2 | 4 / 4 |
| 51 | Sb | [Kr] 5s2 4d10 5p3 | yes | 3 / 3 | 5 / 5 |
| 52 | Te | [Kr] 5s2 4d10 5p4 | yes | 2 / 2 | 6 / 6 |
| 53 | I | [Kr] 5s2 4d10 5p5 | yes | 1 / 1 | 7 / 7 |
| 54 | Xe | [Kr] 5s2 4d10 5p6 | yes | 0 / 0 | 0 / 8 |
| 55 | Cs | [Xe] 6s1 | yes | 1 / 1 | 1 / 1 |
| 56 | Ba | [Xe] 6s2 | yes | 0 / 0 | 2 / 2 |
| 57 | La | [Xe] 6s2 4f1 | no | 1 / 1 | 3 / 3 |
| 58 | Ce | [Xe] 6s2 4f2 | no | 2 / 0 | 4 / 4 |
| 59 | Pr | [Xe] 6s2 4f3 | yes | 3 / 3 | 5 / 5 |
| 60 | Nd | [Xe] 6s2 4f4 | yes | 4 / 4 | 6 / 4 |
| 61 | Pm | [Xe] 6s2 4f5 | yes | 5 / 5 | 7 / 3 |
| 62 | Sm | [Xe] 6s2 4f6 | yes | 6 / 6 | 8 / 3 |
| 63 | Eu | [Xe] 6s2 4f7 | yes | 7 / 7 | 9 / 3 |
| 64 | Gd | [Xe] 6s2 4f8 | no | 6 / 8 | 8 / 3 |
| 65 | Tb | [Xe] 6s2 4f9 | yes | 5 / 5 | 7 / 4 |
| 66 | Dy | [Xe] 6s2 4f10 | yes | 4 / 4 | 6 / 4 |
| 67 | Ho | [Xe] 6s2 4f11 | yes | 3 / 3 | 5 / 3 |
| 68 | Er | [Xe] 6s2 4f12 | yes | 2 / 2 | 4 / 3 |
| 69 | Tm | [Xe] 6s2 4f13 | yes | 1 / 1 | 3 / 3 |
| 70 | Yb | [Xe] 6s2 4f14 | yes | 0 / 0 | 2 / 3 |

| Z | El. | Predicted configuration | Config. | Unpaired | Highest ox. |
|---|---|---|---|---|---|
| 71 | Lu | [Xe] 6s2 4f14 5d1 | yes | 1 / 1 | 3 / 3 |
| 72 | Hf | [Xe] 6s2 4f14 5d2 | yes | 2 / 2 | 4 / 4 |
| 73 | Ta | [Xe] 6s2 4f14 5d3 | yes | 3 / 3 | 5 / 5 |
| 74 | W | [Xe] 6s2 4f14 5d4 | yes | 4 / 4 | 6 / 6 |
| 75 | Re | [Xe] 6s2 4f14 5d5 | yes | 5 / 5 | 7 / 7 |
| 76 | Os | [Xe] 6s2 4f14 5d6 | yes | 4 / 4 | 6 / 8 |
| 77 | Ir | [Xe] 6s2 4f14 5d7 | yes | 3 / 3 | 5 / 9 |
| 78 | Pt | [Xe] 6s2 4f14 5d8 | no | 2 / 2 | 4 / 6 |
| 79 | Au | [Xe] 6s2 4f14 5d9 | no | 1 / 1 | 3 / 5 |
| 80 | Hg | [Xe] 6s2 4f14 5d10 | yes | 0 / 0 | 2 / 2 |
| 81 | Tl | [Xe] 6s2 4f14 5d10 6p1 | yes | 1 / 1 | 3 / 3 |
| 82 | Pb | [Xe] 6s2 4f14 5d10 6p2 | yes | 2 / — | 4 / 4 |
| 83 | Bi | [Xe] 6s2 4f14 5d10 6p3 | yes | 3 / 3 | 5 / 5 |
| 84 | Po | [Xe] 6s2 4f14 5d10 6p4 | yes | 2 / 2 | 6 / 6 |
| 85 | At | [Xe] 6s2 4f14 5d10 6p5 | yes | 1 / 1 | 7 / 7 |
| 86 | Rn | [Xe] 6s2 4f14 5d10 6p6 | yes | 0 / 0 | 0 / 6 |
| 87 | Fr | [Rn] 7s1 | yes | 1 / 1 | 1 / 1 |
| 88 | Ra | [Rn] 7s2 | yes | 0 / 0 | 2 / 2 |
| 89 | Ac | [Rn] 7s2 5f1 | no | 1 / 1 | 3 / 3 |
| 90 | Th | [Rn] 7s2 5f2 | no | 2 / 2 | 4 / 4 |
| 91 | Pa | [Rn] 7s2 5f3 | no | 3 / — | 5 / 5 |
| 92 | U | [Rn] 7s2 5f4 | no | 4 / — | 6 / 6 |
| 93 | Np | [Rn] 7s2 5f5 | no | 5 / — | 7 / 7 |
| 94 | Pu | [Rn] 7s2 5f6 | yes | 6 / 6 | 8 / 8 |
| 95 | Am | [Rn] 7s2 5f7 | yes | 7 / 7 | 9 / 7 |
| 96 | Cm | [Rn] 7s2 5f8 | no | 6 / 8 | 8 / 6 |
| 97 | Bk | [Rn] 7s2 5f9 | yes | 5 / 5 | 7 / 5 |
| 98 | Cf | [Rn] 7s2 5f10 | yes | 4 / 4 | 6 / 5 |
| 99 | Es | [Rn] 7s2 5f11 | yes | 3 / 3 | 5 / 4 |
| 100 | Fm | [Rn] 7s2 5f12 | yes | 2 / 2 | 4 / 3 |
| 101 | Md | [Rn] 7s2 5f13 | yes | 1 / 1 | 3 / 3 |
| 102 | No | [Rn] 7s2 5f14 | yes | 0 / 0 | 2 / 3 |
| 103 | Lr | [Rn] 7s2 5f14 6d1 | no | 1 / 1 | 3 / 3 |
| 104 | Rf | [Rn] 7s2 5f14 6d2 | yes | 2 / 2 | 4 / — |
| 105 | Db | [Rn] 7s2 5f14 6d3 | yes | 3 / 3 | 5 / — |

| Z | El. | Predicted configuration | Config. | Unpaired | Highest ox. |
|---|---|---|---|---|---|
| 106 | Sg | [Rn] 7s2 5f14 6d4 | yes | 4 / — | 6 / — |
| 107 | Bh | [Rn] 7s2 5f14 6d5 | yes | 5 / — | 7 / — |
| 108 | Hs | [Rn] 7s2 5f14 6d6 | yes | 4 / — | 6 / — |
| 109 | Mt | [Rn] 7s2 5f14 6d7 | yes | 3 / — | 5 / — |
| 110 | Ds | [Rn] 7s2 5f14 6d8 | no | 2 / — | 4 / — |
| 111 | Rg | [Rn] 7s2 5f14 6d9 | no | 1 / — | 3 / — |
| 112 | Cn | [Rn] 7s2 5f14 6d10 | yes | 0 / — | 2 / — |
| 113 | Nh | [Rn] 7s2 5f14 6d10 7p1 | yes | 1 / — | 3 / — |
| 114 | Fl | [Rn] 7s2 5f14 6d10 7p2 | yes | 2 / — | 4 / — |
| 115 | Mc | [Rn] 7s2 5f14 6d10 7p3 | yes | 3 / — | 5 / — |
| 116 | Lv | [Rn] 7s2 5f14 6d10 7p4 | yes | 2 / — | 6 / — |
| 117 | Ts | [Rn] 7s2 5f14 6d10 7p5 | yes | 1 / — | 7 / — |
| 118 | Og | [Rn] 7s2 5f14 6d10 7p6 | yes | 0 / — | 0 / — |

# Appendix C — The Programs

Every number in this book comes from the programs below. They run with Python 3, numpy, networkx and the public mendeleev package; RDKit is used once, to check proline. Anyone can run them and get the same numbers.

## periodiek.py — all 118 elements: configuration, period, block, magnetism, oxidation, ionisation, radius

```
"""The complete periodic table from the vacuum.net readings, element by element (Z = 1..118).

Predictions use only the readings of the book:
 A1-A3  places, capacities, filling order n + l          -> configuration, period, block
 A5     N3 inside a set: same direction first, pair after half -> unpaired electrons of the atom
 A6     easiest loss right after a new set opens / first forced pairing -> IE1 drop between Z-1 and
Z
 A7/M1  open passages = distance to nearest closure, per set:  max oxidation state
        = s passages + min(k, cap - k) of the last open d or f set (+ p passages for p-block)
 R      radius: more passages in the same depth pull in; a new depth (new s set) jumps out
Measured data: mendeleev package (NIST-based) — configurations, ground levels, IE1, oxidation
states, radii.
"""
import json, re, warnings
warnings.filterwarnings("ignore")
from mendeleev.fetch import fetch_table
from mendeleev import element

L = "spdf"; cap = {l: 2 * (2 * l + 1) for l in range(4)}
order = sorted(((n, l) for n in range(1, 8) for l in range(min(n, 4))), key=lambda t: (t[0] + t[1],
t[0]))
el = fetch_table("elements").set_index("atomic_number")
ie = fetch_table("ionizationenergies")
neu = ie[ie.ion_charge == 0].drop_duplicates("atomic_number").set_index("atomic_number")

def predicted(Z):
    conf, left = {}, Z
    for n, l in order:
        if left <= 0: break
        k = min(left, cap[l]); conf[(n, l)] = k; left -= k
    return conf

CORE = {"He": 2, "Ne": 10, "Ar": 18, "Kr": 36, "Xe": 54, "Rn": 86}
def parse(ec):
    conf = {}
    for tok in ec.split():
        if tok.startswith("["): conf.update(predicted(CORE[tok.strip("[]")])); continue
        conf[(int(tok[0]), L.index(tok[1]))] = int(tok[2:]) if len(tok) > 2 else 1
    return {k: v for k, v in conf.items() if v}

def unpaired(conf):  # A5 (N3 / Hund) per set
    return sum(k if k <= 2 * l + 1 else 2 * (2 * l + 1) - k for (n, l), k in conf.items())

def short(conf):
    last_noble = max([z for z in CORE.values() if z < sum(conf.values()) and all(predicted(z).get(s,
0) <= conf.get(s, 0) for s in predicted(z))] + [0])
    core = predicted(last_noble)
    rest = [(s, k) for s, k in sorted(conf.items(), key=lambda t: order.index(t[0])) if k !=
core.get(s, 0) or s not in core]
    name = {v: k for k, v in CORE.items()}.get(last_noble)
    return (f"[{name}] " if name else "") + " ".join(f"{n}{L[l]}{k}" for (n, l), k in rest)

def last_set(conf):
    return max(conf, key=lambda s: order.index(s))

def max_ox_pred(conf, Z):
    if Z in CORE.values() or Z == 118: return 0          # standing closure (noble gas)
    if Z == 1: return 1
    s_top = max(n for (n, l) in conf if l == 0)
    s = conf.get((s_top, 0), 0)
    p = conf.get((s_top, 1), 0)
    if p: return s + p                                    # p-block: all outer passages
    opens = [(n, l) for (n, l), k in conf.items() if l >= 2 and k < cap[l]]
    if not opens: return s if not any(l >= 2 and (n, l) == last_set(conf) for (n, l) in conf) else s
    n, l = max(opens, key=lambda t: order.index(t))
    k = conf[(n, l)]
    return s + min(k, cap[l] - k)

OXW = json.load(open("ox_wiki.json"))
def max_ox_group(conf, Z):
```

```
    """REJECTED (tested, 51/115, buggy for p-block after a d core; not used in the book).
    Rule B: give up every passage above the last closed noble core (s + d + p, f counted only
    as the one f/d passage that crosses), never more than 8 = one full s+p closure."""
    if Z in CORE.values(): return 0
    core = max([z for z in CORE.values() if z < Z] + [0])
    k = Z - core
    if any(l == 3 and v for (n, l), v in conf.items() if (n, l) not in predicted(core)):
        k = 3  # f passages sit inside; only s2 + one cross over
    return min(k, 8)

def ground_unpaired(level):
    m = re.match(r"(\d+)[SPDFGHI]", str(level))
    return int(m.group(1)) - 1 if m else None

rows = []
for Z in range(1, 119):
    sym = el.loc[Z, "symbol"]
    pc = predicted(Z); real = parse(el.loc[Z, "electronic_configuration"])
    r = {"Z": Z, "sym": sym, "name": el.loc[Z, "name"], "real_conf": el.loc[Z,
"electronic_configuration"], "conf_pred": short(pc), "conf_ok": real == {k: v for k, v in pc.items()
if v},
         "period_pred": max(n for n, l in pc), "period": int(el.loc[Z, "period"]),
         "block_pred": L[last_set(pc)[1]], "block": el.loc[Z, "block"],
         "unp_pred": unpaired(pc), "unp_meas": ground_unpaired(neu.loc[Z, "ground_level"]) if Z in
neu.index else None,
         "ie1": float(neu.loc[Z, "ionization_energy"]) if Z in neu.index else None}
    r["ox_max_pred"] = max_ox_pred(pc, Z)
    r["ox_max_pred_b"] = max_ox_group(pc, Z)
    r["ox_max_meas"] = OXW["max"].get(sym)
    rad = el.loc[Z, "covalent_radius_pyykko"]
    r["radius"] = float(rad) if rad == rad else None
    rows.append(r)

def score(key_p, key_m, subset=None):
    rr = [r for r in rows if r[key_m] is not None and (subset is None or subset(r))]
    return sum(r[key_p] == r[key_m] for r in rr), len(rr)

res = {}
res["configuration"] = (sum(r["conf_ok"] for r in rows), 118)
res["period"] = score("period_pred", "period")
res["block"] = score("block_pred", "block")
res["unpaired_all"] = score("unp_pred", "unp_meas")
for b in "spdf":
    res[f"unpaired_{b}"] = score("unp_pred", "unp_meas", lambda r, b=b: r["block"] == b)
res["unpaired_when_conf_ok"] = score("unp_pred", "unp_meas", lambda r: r["conf_ok"])
for b in "spdf":
    res[f"oxmax_{b}"] = score("ox_max_pred", "ox_max_meas", lambda r, b=b: r["block"] == b and
r["Z"] not in CORE.values())
res["oxmax_noble"] = score("ox_max_pred", "ox_max_meas", lambda r: r["Z"] in CORE.values())
for b in "spdf":
    res[f"oxmaxB_{b}"] = score("ox_max_pred_b", "ox_max_meas", lambda r, b=b: r["block"] == b and
r["Z"] not in CORE.values())
res["oxmaxA_all"] = score("ox_max_pred", "ox_max_meas")
res["oxmaxB_all"] = score("ox_max_pred_b", "ox_max_meas")
res["oxmax_A_or_B"] = (sum(r["ox_max_meas"] in (r["ox_max_pred"], r["ox_max_pred_b"]) for r in rows
if r["ox_max_meas"] is not None), sum(r["ox_max_meas"] is not None for r in rows))

# IE1 drops (A6): predicted where Z opens a new set (first passage of a new (n,l)) or makes the
first forced pairing in a p set
def opens_or_pairs(Z):
    a, b = predicted(Z - 1), predicted(Z)
    new = [s for s in b if s not in a]
    if new: return True
    s = last_set(b); n, l = s
    return l == 1 and b[s] == 2 * l + 2
ie_ok = ie_n = 0; ie_by = {"s": [0, 0], "p": [0, 0], "d": [0, 0], "f": [0, 0]}; ie_miss = []
for Z in range(2, 119):
    a, b = rows[Z - 2]["ie1"], rows[Z - 1]["ie1"]
    if a is None or b is None: continue
    pred_drop = opens_or_pairs(Z); meas_drop = b < a
    ok = pred_drop == meas_drop
    ie_ok += ok; ie_n += 1
    blk = rows[Z - 1]["block"]; ie_by[blk][0] += ok; ie_by[blk][1] += 1
    if not ok: ie_miss.append(rows[Z - 1]["sym"])
res["ie1_direction"] = (ie_ok, ie_n); res["ie1_by_block"] = ie_by

# Radius (R): drop within a depth, jump at new period
rad_ok = rad_n = 0; rad_by = {"s": [0, 0], "p": [0, 0], "d": [0, 0], "f": [0, 0]}
for Z in range(2, 119):
    a, b = rows[Z - 2]["radius"], rows[Z - 1]["radius"]
    if a is None or b is None or Z in (2,): continue
    new_period = rows[Z - 1]["period_pred"] > rows[Z - 2]["period_pred"]
    if not new_period and rows[Z - 2]["Z"] in CORE.values(): continue
    pred_up = new_period; meas_up = b > a
    if b == a: continue
    ok = pred_up == meas_up; rad_ok += ok; rad_n += 1
    blk = rows[Z - 1]["block"]; rad_by[blk][0] += ok; rad_by[blk][1] += 1
```

```
res["radius_direction"] = (rad_ok, rad_n); res["radius_by_block"] = rad_by

for k, v in res.items(): print(f"{k:24s} {v}")
print("IE1 misses:", " ".join(ie_miss))
print("unpaired misses:", " ".join(f"{r['sym']}({r['unp_pred']}/{r['unp_meas']})" for r in rows if
r["unp_meas"] is not None and r["unp_pred"] != r["unp_meas"]))
print("oxmax B misses:", " ".join(f"{r['sym']}({r['ox_max_pred_b']}/{r['ox_max_meas']})" for r in
rows if r["ox_max_meas"] is not None and r["ox_max_pred_b"] != r["ox_max_meas"]))
print("oxmax A misses:", " ".join(f"{r['sym']}({r['ox_max_pred']}/{r['ox_max_meas']})" for r in rows
if r["ox_max_meas"] is not None and r["ox_max_pred"] != r["ox_max_meas"]))
json.dump({"rows": rows, "res": res, "ie_miss": ie_miss}, open("periodiek.json", "w"), indent=1,
default=str)
```

# atomen.py — capacities, order, periods, first tests of ionisation and oxidation

```
"""Atoms from the vacuum.net theory, tested against element data (mendeleev package).

A1 Places of depth l: the balanced-ternary integers -l..l, so 2l+1 places.
A2 Each place holds two directions (N3: +1 / -1): capacity 2(2l+1) = 2, 6, 10, 14.
A3 Cost of a place set (n, l): inner closed rings of the same kind (n-l-1) plus its
   own number of places (2l+1)  ->  n + l (up to a constant). Ties: fewer inner rings first,
   i.e. lower n. This is the Madelung order.
A4 A period ends where the axis set (l=1) closes: a standing closure (noble gas).
A5 Within a set, passages go the same direction first (N3); pairing starts after half.
A6 Ionisation is easiest right after a new set opens, and right after the first forced pairing.
A7 Oxidation states: give up all k open passages (+k) or fill to closure (k - P).
"""
import json, warnings
warnings.filterwarnings("ignore")
from mendeleev.fetch import fetch_table
el = fetch_table("elements").set_index("atomic_number")

L = "spdf"
# A1-A3
cap = {l: 2 * (2 * l + 1) for l in range(4)}
order = sorted(((n, l) for n in range(1, 8) for l in range(min(n, 4))), key=lambda t: (t[0] + t[1],
t[0]))
out = {"capacities": {L[l]: c for l, c in cap.items()}}
print("A2 capacities:", out["capacities"])
print("A3 order:", " ".join(f"{n}{L[l]}" for n, l in order))

# A4: periods
periods, cur = [], 0
for n, l in order:
    cur += cap[l]
    if l == 1 or (n, l) == (1, 0):
        periods.append(cur); cur = 0
periods = periods[:7]
print("A4 period lengths:", periods)
out["periods"] = periods

# predicted configurations vs real (Z = 1..118)
def predicted(Z):
    conf, left = {}, Z
    for n, l in order:
        if left <= 0: break
        k = min(left, cap[l]); conf[(n, l)] = k; left -= k
    return conf

def parse(ec):
    core = {"He": 2, "Ne": 10, "Ar": 18, "Kr": 36, "Xe": 54, "Rn": 86}
    conf = {}
    for tok in ec.split():
        if tok.startswith("["):
            for z_n, l_n in [(1,0),(2,0),(2,1),(3,0),(3,1),(4,0),(3,2),(4,1),(5,0),(4,2),(5,1),
(6,0),(4,3),(5,2),(6,1)]:
                pass
            gas = tok.strip("[]"); conf.update(predicted(core[gas])); continue
        n = int(tok[0]); l = L.index(tok[1]); k = int(tok[2:]) if len(tok) > 2 else 1
        conf[(n, l)] = k
    return {k: v for k, v in conf.items() if v}

exceptions = []
for Z in range(1, 119):
    ec = el.loc[Z, "electronic_configuration"]
    if not isinstance(ec, str): continue
    if parse(ec) != {k: v for k, v in predicted(Z).items() if v}:
        exceptions.append(el.loc[Z, "symbol"])
print(f"A3 configurations: {118 - len(exceptions)}/118 exact; exceptions ({len(exceptions)}):", "
".join(exceptions))
out["config_exact"] = 118 - len(exceptions); out["config_exceptions"] = exceptions
```

```
# A6: ionisation dips in the p-block (periods 2..6): group 13 below 2, group 16 below 15
ie = fetch_table("ionizationenergies")
ie1 = ie[ie.ion_charge == 0].drop_duplicates("atomic_number").set_index("atomic_number")
["ionization_energy"]
dips = []
rows = {2: (4, 5, 7, 8), 3: (12, 13, 15, 16), 4: (30, 31, 33, 34), 5: (48, 49, 51, 52), 6: (80, 81,
83, 84)}
hit = 0
for p, (g2, g13, g15, g16) in rows.items():
    a = ie1[g13] < ie1[g2]; b = ie1[g16] < ie1[g15]
    hit += a + b
    dips.append((p, el.loc[g13, "symbol"], round(ie1[g2], 2), round(ie1[g13], 2), bool(a),
                 el.loc[g16, "symbol"], round(ie1[g15], 2), round(ie1[g16], 2), bool(b)))
for d in dips: print("A6", d)
print(f"A6 dips predicted and found: {hit}/10")
out["ie_dips"] = dips; out["ie_hits"] = hit

# A7: oxidation states, main groups 1,2,13-17, periods 2-6
groups = {1: 1, 2: 2, 13: 3, 14: 4, 15: 5, 16: 6, 17: 7}
ox_rows, max_ok, min_ok, n_max, n_min = [], 0, 0, 0, 0
for Z in range(3, 87):
    g = el.loc[Z, "group_id"]
    if g not in groups or Z in (1, 2): continue
    k = groups[int(g)]
    states = [s for s in el.loc[Z, "oxistates"] if True] if False else None
from mendeleev import element
for Z in range(3, 87):
    e = element(Z)
    if e.group_id not in groups: continue
    k = groups[e.group_id]
    try: allst = [o.oxidation_state for o in e.oxidation_states()]
    except Exception: allst = e.oxistates
    if not allst: continue
    n_max += 1; mx = max(allst); okmax = (mx == k); max_ok += okmax
    row = [e.symbol, k, mx, okmax]
    if k >= 4:
        n_min += 1; mn = min(allst); okmin = (mn == k - 8); min_ok += okmin; row += [mn, okmin]
    ox_rows.append(row)
print(f"A7 highest state = +k: {max_ok}/{n_max};  lowest state = k-8 (groups 14-17): {min_ok}/
{n_min}")
print("A7 misses:", [r for r in ox_rows if not r[3] or (len(r) > 4 and not r[5])])
out["ox"] = {"max_ok": max_ok, "n_max": n_max, "min_ok": min_ok, "n_min": n_min,
             "misses": [r for r in ox_rows if not r[3] or (len(r) > 4 and not r[5])]}
json.dump(out, open("atomen.json", "w"), indent=1, default=str)
```

# molecuul.py — closed molecules, cube angles

```
"""Small molecules generated from the closure rule of the vacuum.net theory.

Rules used (Ninth Edition reading):
 1. An atom on period P at position k keeps open passages v = min(k, P-k):
    the distance to the nearest closure (full or empty period). Noble gas: v=0 (standing closure).
 2. A bond is a meeting closure (x, -x): one open passage of each atom, carry 0.
 3. A molecule is a connected set of atoms in which every open passage is closed. Tension zero.
 4. Geometry from the cube (8 nodes): directions are cube vertices.
"""
import itertools, math
import numpy as np

# Rule 1: valence from period position
periods = {"H": (1, 2), "He": (2, 2), "C": (4, 8), "N": (5, 8), "O": (6, 8), "F": (7, 8), "Ne": (8,
8)}
val = {el: min(k, P - k) for el, (k, P) in periods.items()}
print("open passages:", val)

def molecules(heavy_max=2, h_max=6):
    """Enumerate closed connected bond graphs: heavy atoms C,N,O,F (+H)."""
    found = set()
    heavy_types = ["C", "N", "O", "F"]
    for nh in range(1, heavy_max + 1):
        for heavy in itertools.combinations_with_replacement(heavy_types, nh):
            # bonds between heavy atoms: multiplicity 0..3 for each pair
            pairs = list(itertools.combinations(range(nh), 2))
            for mult in itertools.product(range(4), repeat=len(pairs)):
                used = [0] * nh
                for (i, j), m in zip(pairs, mult):
                    used[i] += m; used[j] += m
                rest = [val[heavy[i]] - used[i] for i in range(nh)]
                if any(r < 0 for r in rest):
                    continue
                # connectivity of heavy skeleton
                if nh > 1:
                    adj = {i: set() for i in range(nh)}
                    for (i, j), m in zip(pairs, mult):
```

```
                        if m: adj[i].add(j); adj[j].add(i)
                    seen, stack = {0}, [0]
                    while stack:
                        for n in adj[stack.pop()]:
                            if n not in seen: seen.add(n); stack.append(n)
                    if len(seen) < nh:
                        continue
                nH = sum(rest)  # every remaining passage closes with one H
                if nH > h_max:
                    continue
                counts = {}
                for el in heavy: counts[el] = counts.get(el, 0) + 1
                if nH: counts["H"] = nH
                bonds = tuple(sorted(mult))
                order = (["C","H"] + sorted(e for e in counts if e not in "CH")) if "C" in counts
else sorted(counts)
                formula = "".join(f"{el}{counts[el] if counts[el] > 1 else ''}" for el in order if
el in counts)
                found.add((formula, bonds))
    return found

mols = molecules()
mols.add(("H2", ()))
names = sorted({f for f, _ in mols})
print(f"\n{len(names)} formulas generated:")
print(", ".join(names))

known = {"H2","CH4","H3N","H2O","FH","C2H6","C2H4","C2H2","N2","F2","CHN","CH2O","CH4O",
"CH3F","H4N2","H2N2","H2O2","CH5N","CH3N","F3N","FHO","FH2N","HNO","H3NO","O2"}
print("\nnot in my textbook list (check by hand):",
      [n for n in names if n not in known])

# Rule 4: angles from cube vertices
v = np.array(list(itertools.product((-1, 1), repeat=3)), float)
ang = lambda a, b: math.degrees(math.acos(max(-1.0, min(1.0, np.dot(a, b) / np.linalg.norm(a) /
np.linalg.norm(b)))))
tet = [v[0], v[3], v[5], v[6]]  # alternate vertices: inscribed tetrahedron
print("\nangle 4 directions (alternate cube vertices):", round(ang(tet[0], tet[1]), 2))
print("angle 2 directions (opposite vertices):      ", round(ang(v[0], v[7]), 2))
# hexagon: 6 vertices perpendicular to body diagonal; three alternate ones lie 120 apart in
projection
d = np.array([1, 1, 1]) / math.sqrt(3)
hexv = [x for x in v if abs(np.dot(x, d)) < 1.5]
proj = [x - np.dot(x, d) * d for x in hexv]
print("angle 3 directions (hexagon around diagonal): ", round(ang(proj[0], proj[3]) if False else
min(
    ang(proj[i], proj[j]) for i in range(6) for j in range(i + 1, 6) if ang(proj[i], proj[j]) > 90),
2))

real = {"CH4": 109.47, "NH3": 107.8, "H2O": 104.5, "CO2": 180.0, "C2H4 (HCH)": 117.4, "HCN": 180.0}
pred = {"CH4": 109.47, "NH3": 109.47, "H2O": 109.47, "CO2": 180.0, "C2H4 (HCH)": 120.0, "HCN":
180.0}
print("\nmolecule   predicted  measured  difference")
for k in real:
    print(f"{k:11s} {pred[k]:8.2f} {real[k]:9.2f} {pred[k]-real[k]:+8.2f}")
```

# diatomen.py — magnetism and bond order of diatomic molecules

```
"""Beyond Lewis: diatomic molecules from the cube, the meeting rule and N3.

Readings (vacuum.net, Ninth Edition):
 - An atom of period 2 has one standing place (centre, s) and three axes (the cube's 3 axes, p).
 - Two atoms share places. Per shared place there are two combinations:
     meeting  (x, -x)  -> closes, lower     ("bonding")
     open     (x,  x)  -> tension, higher   ("antibonding")
 - The bond picks one axis. The two other axes are equivalent: a degenerate pair.
 - N3: the first passage fixes the direction. In a degenerate pair, a later passage
   leaves the way the first did (+1, same sign) unless forced to pair. -> parallel first.
Counted: electrons (passages), not valences. That is the step past Lewis.
"""
VAL = {"B": 3, "C": 4, "N": 5, "O": 6, "F": 7}

def levels(pi_below_sigma):
    # (name, degeneracy, bonding?)
    s = [("s", 1, True), ("s*", 1, False)]
    p = [("pi", 2, True), ("sig", 1, True)] if pi_below_sigma else [("sig", 1, True), ("pi", 2,
True)]
    return s + p + [("pi*", 2, False), ("sig*", 1, False)]

def fill(n, pi_below_sigma):
    unpaired, bond, anti = 0, 0, 0
    for name, deg, bonding in levels(pi_below_sigma):
        k = min(n, 2 * deg); n -= k
        # N3: same sign first across the degenerate places, pair only when forced
```

```
        up = k if k <= deg else 2 * deg - k
        unpaired += up
        if bonding: bond += k
        else: anti += k
    return unpaired, (bond - anti) / 2

cases = {  # molecule: (electrons, unpaired measured, bond length in Angstrom)
    "B2": (6, 2, 1.590), "C2": (8, 0, 1.243), "N2": (10, 0, 1.098), "O2": (12, 2, 1.208),
    "F2": (14, 0, 1.412), "CO": (10, 0, 1.128), "NO": (11, 1, 1.151), "CN": (9, 1, 1.172),
    "O2+": (11, 1, 1.116), "O2-": (13, 1, 1.33),
}
print(f"{'mol':5s} {'e':>3s} | {'unpaired':>8s} {'meas':>4s} | {'order':>5s} {'length':>6s} |
ordering A (sig below pi) ok?")
rowsA, rowsB = [], []
for m, (e, meas, L) in cases.items():
    uB, oB = fill(e, True)   # pi below sigma
    uA, oA = fill(e, False)  # sigma below pi
    rowsA.append(uA == meas); rowsB.append(uB == meas)
    print(f"{m:5s} {e:3d} | B:{uB:2d} A:{uA:2d} {meas:4d} | {oB:5.1f} {L:6.3f} | A {'ok' if uA==meas
else 'WRONG'}  B {'ok' if uB==meas else 'WRONG'}")
print(f"\nmagnetism right: ordering A {sum(rowsA)}/{len(rowsA)}, ordering B {sum(rowsB)}/
{len(rowsB)}")

# Does bond order rank bond length? (higher order -> shorter)
import itertools
pairs = list(itertools.combinations(cases, 2))
agree = tie = 0
for a, b in pairs:
    oa, ob = fill(cases[a][0], True)[1], fill(cases[b][0], True)[1]
    la, lb = cases[a][2], cases[b][2]
    if oa == ob: tie += 1
    elif (oa > ob) == (la < lb): agree += 1
print(f"bond order vs length: {agree} of {len(pairs)-tie} untied pairs in the right order ({tie}
ties)")
```

# niveauvolgorde.py — ring rule, periods 2 and 3

```
"""Deriving the level order (pi vs sigma) from the ring closure, and testing it.

Ring rule (T7: x, x, x closes and carries one passage to the next scale):
 - The three axes of an atom fill with parallel passages first (N3).
 - With p <= 3 passages the axis-ring is not yet past closure. The standing place (s)
   and the bond axis are still one level: they mix, the bond axis is pushed up.
   -> pi below sigma.
 - With p >= 4 the ring has closed and carried. The axes sit on their own level.
   -> sigma below pi.
 Crossover predicted between N (p = 3, the ring itself) and O (p = 4).
 Heteronuclear: use the mean number of p-passages of the two atoms.
"""
import importlib.util, sys
spec = importlib.util.spec_from_file_location("d", sys.argv[1] if len(sys.argv) > 1 else
"diatomen.py")
src = open("diatomen.py").read().split("cases = {")[0]
ns = {}; exec(src, ns); fill = ns["fill"]

def p_passages(val_e): return val_e - 2   # s holds 2, the rest sits on the axes

VE = {"B": 3, "C": 4, "N": 5, "O": 6, "F": 7, "Al": 3, "Si": 4, "P": 5, "S": 6, "Cl": 7}

def predict(a, b, charge=0):
    e = VE[a] + VE[b] - charge
    mean_p = (p_passages(VE[a]) + p_passages(VE[b])) / 2
    pi_below = mean_p <= 3
    return fill(e, pi_below)[0], ("pi<sig" if pi_below else "sig<pi")

tests = [  # (a, b, charge, measured unpaired, ground state, period)
    ("B", "B", 0, 2, "3Sg-", 2), ("C", "C", 0, 0, "1Sg+", 2), ("N", "N", 0, 0, "1Sg+", 2),
    ("O", "O", 0, 2, "3Sg-", 2), ("F", "F", 0, 0, "1Sg+", 2), ("C", "O", 0, 0, "1S+", 2),
    ("N", "O", 0, 1, "2Pi", 2), ("C", "N", 0, 1, "2S+", 2), ("O", "O", 1, 1, "2Pg", 2), ("O", "O",
-1, 1, "2Pg", 2),
    # independent test: period 3, not used to set the rule
    ("Al", "Al", 0, 2, "3Pu", 3), ("Si", "Si", 0, 2, "3Sg-", 3), ("P", "P", 0, 0, "1Sg+", 3),
    ("S", "S", 0, 2, "3Sg-", 3), ("Cl", "Cl", 0, 0, "1Sg+", 3),
]
for per in (2, 3):
    ok = 0; rows = [t for t in tests if t[5] == per]
    print(f"\nperiod {per}")
    for a, b, q, meas, gs, _ in rows:
        u, order = predict(a, b, q)
        name = f"{a}{b if b != a else '2'}" + ("+" if q == 1 else "-" if q == -1 else "")
        ok += (u == meas)
        print(f"  {name:6s} {order:7s} predicted {u}  measured {meas} ({gs})  {'ok' if u == meas
else 'WRONG'}")
    print(f"  right: {ok}/{len(rows)}")
```

# periodes.py — inner-ring rule, periods 2–5, node identity

```
"""Period 2 versus period 3 and deeper: the inner ring on the axes.

Reading:
 - An orbital (n, l) has n - l - 1 radial nodes.
 - The number of closed inner shells of the same kind (same l) below it is also n - l - 1.
 - In the net: each closed inner ring of the same kind is carried up as one passage.
   The valence passage is then taken relative to it (N3) and mirrored once per inner ring.
   Mirror = negation = a sign change = a node.
 - Period 2 axes (2p) have no inner axis-ring: they are free. Strong mixing with the
   standing place (2s): pi below sigma until the ring closes (rule of section 11).
 - Period 3 and deeper axes stand on a closed inner axis-ring: mixing is weak.
   sigma and pi are then near one level: three equivalent places, filled by N3,
   until the ring closes; after that sigma below pi.
Fitted on: Si2 (section 11). Tested blind on: periods 4 and 5.
"""
def nodes(n, l): return n - l - 1
def inner_same_kind(n, l): return sum(1 for m in range(l + 1, n))
assert all(nodes(n, l) == inner_same_kind(n, l) for n in range(1, 8) for l in range(n))
print("nodes = inner closed rings of the same kind: identical for all n<=7 (counting identity)")

def unpaired_p_block(p_total, period):
    """p_total = electrons in the sigma_p, pi, pi*, sigma* manifold of a homonuclear dimer."""
    # bonding manifold: sigma (1 place) + pi (2 places); antibonding: pi* (2) + sigma* (1)
    per_atom = p_total / 2
    if per_atom > 3:          # ring closed: sigma below pi, then pi*, sigma*
        levels = [1, 2, 2, 1]
    elif period == 2:         # strong mixing: pi below sigma
        levels = [2, 1, 2, 1]
    else:                     # weak mixing: sigma and pi one level of 3 places
        levels = [3, 2, 1]
    n, up = p_total, 0
    for deg in levels:
        k = min(n, 2 * deg); n -= k
        up += k if k <= deg else 2 * deg - k
    return up

groups = {13: 1, 14: 2, 15: 3, 16: 4, 17: 5}  # p-electrons per atom
data = {  # period: [(symbol, group, measured unpaired, ground state)]
    2: [("B2", 13, 2, "3Sg-"), ("C2", 14, 0, "1Sg+"), ("N2", 15, 0, "1Sg+"), ("O2", 16, 2, "3Sg-"),
("F2", 17, 0, "1Sg+")],
    3: [("Al2", 13, 2, "3Pu"), ("Si2", 14, 2, "3Sg-"), ("P2", 15, 0, "1Sg+"), ("S2", 16, 2, "3Sg-"),
("Cl2", 17, 0, "1Sg+")],
    4: [("Ga2", 13, 2, "3Pu"), ("Ge2", 14, 2, "3Sg-"), ("As2", 15, 0, "1Sg+"), ("Se2", 16, 2,
"3Sg-"), ("Br2", 17, 0, "1Sg+")],
    5: [("In2", 13, 2, "3Pu"), ("Sn2", 14, 2, "3Sg-"), ("Sb2", 15, 0, "1Sg+"), ("Te2", 16, 2,
"3Sg-"), ("I2", 17, 0, "1Sg+")],
}
for per, rows in data.items():
    tag = "rule set here" if per == 2 else "fitted on Si2" if per == 3 else "blind"
    ok = 0
    print(f"\nperiod {per} ({tag})")
    for sym, g, meas, gs in rows:
        u = unpaired_p_block(2 * groups[g], per)
        ok += u == meas
        print(f"  {sym:4s} predicted {u}  measured {meas} ({gs})  {'ok' if u == meas else 'WRONG'}")
    print(f"  right: {ok}/{len(rows)}")
```

# bindingslengte.py — shortening ratio Q

```
"""A number without a unit: how bond length shrinks with bond order.

Unit-free quantity per bond series (single, double, triple):
    Q = (L1 - L3) / (L1 - L2)
A unit drops out, so a theory of ratios can predict it.

Candidate laws for the shrink s(n) = L1 - Ln, each with one free scale:
  linear     s ~ (n - 1)        -> Q = 2
  harmonic   s ~ (1 - 1/n)      -> Q = 4/3
  scale-step s ~ (1 - r^(n-1)) -> Q depends on r (geometric, N5 as fixed factor per step)
  depth      s ~ log n          -> Q = log 3 / log 2 = log2(3) = 1.58496...
'depth' is the vacuum.net reading: n closures need depth ~ log n (N5, address depth).
Note: the depth law is Pauling's 1947 bond-order law; I knew it beforehand.
"""
import math, statistics

data = {  # bond lengths in angstrom (textbook values, from memory, to be checked)
    "C-C": (1.54, 1.34, 1.20),
    "C-N": (1.47, 1.28, 1.16),
```

```
    "N-N": (1.45, 1.25, 1.10),
    "C-O": (1.43, 1.21, 1.13),
}
laws = {"linear": 2.0, "harmonic": 4 / 3, "depth log2(3)": math.log2(3)}
Q = {k: (a - c) / (a - b) for k, (a, b, c) in data.items()}
for k, q in Q.items():
    print(f"{k}: Q = {q:.3f}")
m = statistics.mean(Q.values()); sd = statistics.stdev(Q.values())
print(f"\nmean Q = {m:.3f}  (sd {sd:.3f}, n = {len(Q)})")
for name, val in laws.items():
    print(f"  {name:14s} predicts {val:.3f}   difference {val - m:+.3f}  ({abs(val - m)/sd:.1f}
sd)")
# geometric scale-step: which r would fit? r^1 shrink... Q = (1 - r^2)/(1 - r) = 1 + r
print(f"  scale-step needs r = {m - 1:.3f} per step; a ternary step r = 1/3 gives Q = {1 +
1/3:.3f}")
# leave-one-out: does the depth law beat the others on each series?
wins = sum(abs(q - math.log2(3)) < min(abs(q - 2), abs(q - 4/3)) for q in Q.values())
print(f"\ndepth law closest in {wins} of {len(Q)} series")
```

# huckel_vsepr.py — aromatic rings, geometry

```
"""Rings and directions.
H1 A closed ring of places has addresses m = -M..M (balanced ternary). Each holds two directions.
   A ring set closes at 2(2M+1) = 2, 6, 10, 14, 18 passages. That is Hückel's 4n+2 (identity: 4n+2 =
2(2n+1)).
G1 Directions from the cube: 2 = opposite vertices (180), 3 = hexagon around a diagonal (120),
   4 = alternate vertices (109.47), 6 = face normals (90). 5 has no cube form.
"""
rings = {  # name: (pi electrons, aromatic measured?)
 "cyclopropenyl cation": (2, True), "cyclobutadiene": (4, False), "cyclopentadienyl anion": (6,
True),
 "benzene": (6, True), "tropylium cation": (6, True), "cyclooctatetraene": (8, False),
 "cyclooctatetraene dianion": (10, True), "naphthalene": (10, True), "[18]annulene": (18, True),
 "pentalene": (8, False), "azulene": (10, True), "pyridine": (6, True), "furan": (6, True),
"thiophene": (6, True),
}
closes = {2 * (2 * M + 1) for M in range(10)}
ok = sum((e in closes) == aro for e, aro in rings.values())
for n, (e, aro) in rings.items():
    print(f"{n:28s} {e:3d}  closes={e in closes}  aromatic={aro}  {'ok' if (e in closes)==aro else
'WRONG'}")
print(f"H1 right: {ok}/{len(rings)}")
geo = {  # molecule: (directions incl. lone pairs, predicted, measured angle)
 "BeCl2(g)": (2, 180.0, 180.0), "CO2": (2, 180.0, 180.0), "BF3": (3, 120.0, 120.0), "SO3": (3,
120.0, 120.0),
 "CH4": (4, 109.47, 109.47), "CCl4": (4, 109.47, 109.47), "NH3": (4, 109.47, 107.8), "H2O": (4,
109.47, 104.5),
 "SF6": (6, 90.0, 90.0), "XeF4": (6, 90.0, 90.0), "PCl5": (5, None, 90.0),
}
for m, (d, p, r) in geo.items():
    print(f"{m:9s} {d} directions  predicted {p}  measured {r}  diff {'' if p is None else round(p-
r,2)}")
```

# isomeren.py — constitutional alkane count

```
"""Counting every alkane C_nH_(2n+2) from the closure rule, with and without mirror forms.

Rules:
 M1  carbon has 4 open passages, hydrogen 1.
 M2  a bond is a meeting (x, -x).
 M3  a molecule is connected and fully closed. For CnH(2n+2) that is: a tree of n carbons,
     each carbon with at most 4 carbon neighbours; hydrogens close the rest.
 G2  (cube) a carbon whose four neighbours are all different sits in one of the cube's two
     tetrahedra. The two are mirror images (negation). Each such carbon carries one sign: + or -.
 Count: distinct closed trees (constitution), and distinct signed trees up to the tree's own
 symmetries (Burnside), mirror images counted separately.
Data: OEIS A000602 (constitutional isomers) and A000628 (with stereoisomers).
"""
import json, sys
import networkx as nx
from networkx.algorithms.isomorphism import GraphMatcher

A000602 = [1, 1, 1, 2, 3, 5, 9, 18, 35, 75, 159, 355, 802, 1858, 4347]
A000628 = [1, 1, 1, 2, 3, 5, 11, 24, 55, 136, 345, 900, 2412, 6563, 18127]
NMAX = int(sys.argv[1]) if len(sys.argv) > 1 else 15

def canon(T, root, parent=None):
    return "(" + "".join(sorted(canon(T, c, root) for c in T[root] if c != parent)) + ")"

def stereocentres(T):
    out = []
```

```
    for v in T:
        d = T.degree(v)
        if d < 3: continue
        branches = [canon(T, c, v) for c in T[v]]
        if len(set(branches)) == d:   # all carbon branches different; with d = 3 the H is the 4th,
also different
            out.append(v)
    return out

def stereo_count(T, centres):
    if not centres: return 1
    idx = {c: i for i, c in enumerate(centres)}
    total = n_aut = 0
    for m in GraphMatcher(T, T).isomorphisms_iter():
        n_aut += 1
        seen, cycles = set(), 0
        for c in centres:
            if c in seen: continue
            cycles += 1; x = c
            while x not in seen:
                seen.add(x); x = m[x]
        total += 2 ** cycles
    return total // n_aut

res = []
for n in range(1, NMAX + 1):
    trees = [nx.empty_graph(1)] if n == 1 else list(nx.nonisomorphic_trees(n))
    closed = [T for T in trees if max(dict(T.degree()).values()) <= 4]
    stereo = sum(stereo_count(T, stereocentres(T)) for T in closed)
    res.append((n, len(closed), A000602[n - 1], stereo, A000628[n - 1]))
    print(f"C{n:<2d}  isomers {len(closed):6d} (known {A000602[n-1]:6d})  with mirror forms
{stereo:6d} (known {A000628[n-1]:6d})", flush=True)
ok1 = sum(r[1] == r[2] for r in res); ok2 = sum(r[3] == r[4] for r in res)
print(f"constitution exact: {ok1}/{len(res)};  with mirror forms exact: {ok2}/{len(res)}")
json.dump(res, open("isomeren.json", "w"))
```

# stereo2.py — alkane count with mirror forms, including pseudo-asymmetric centres

```
"""Stereoisomers without shortcuts: every carbon with three or four carbon neighbours gets a sign
(one of the cube's two tetrahedra). Two signed molecules are the same if their canonical
signed strings agree. A sign only counts where the four ligands differ, *including their own
signs*. That catches the pseudo-asymmetric case: two branches that are mirror images make a
centre stereogenic. Mirror images of the whole molecule are counted separately.
"""
import itertools, json, sys
import networkx as nx
A000628 = [1, 1, 1, 2, 3, 5, 11, 24, 55, 136, 345, 900, 2412, 6563, 18127]
NMAX = int(sys.argv[1]) if len(sys.argv) > 1 else 14

def parity(perm):
    p, s, seen = list(perm), 1, set()
    for i in range(len(p)):
        if i in seen: continue
        j, L = i, 0
        while j not in seen: seen.add(j); j = p[j]; L += 1
        if L % 2 == 0: s = -s
    return s

def string(T, v, parent, sign):
    kids = sorted((string(T, c, v, sign), c) for c in T[v] if c != parent)
    nh = 4 - T.degree(v)
    ligs = ([("P", parent)] if parent is not None else []) + [(s, c) for s, c in kids] + [("H",
None)] * nh
    labels = [l for l, _ in ligs]
    desc = 0
    if v in sign and len(set(labels)) == 4:
        # raw sign is defined for the neighbour order sorted by node id, H last
        raw = sorted([c for _, c in ligs if c is not None]) + [None] * nh
        canon_order = [c for _, c in ligs]
        perm = [raw.index(c) for c in canon_order]
        desc = sign[v] * parity(perm)
    return "(" + {1: "+", -1: "-", 0: ""}[desc] + "".join(s for s, _ in kids) + ")"

def count(T):
    cand = [v for v in T if T.degree(v) >= 3]
    centres = nx.center(T)
    forms = set()
    for signs in itertools.product((1, -1), repeat=len(cand)):
        sg = dict(zip(cand, signs))
        forms.add(min(string(T, r, None, sg) for r in centres))
    return len(forms)
```

```
out = []
for n in range(1, NMAX + 1):
    trees = [nx.empty_graph(1)] if n == 1 else [T for T in nx.nonisomorphic_trees(n) if
max(dict(T.degree()).values()) <= 4]
    c = sum(count(T) for T in trees)
    out.append((n, c, A000628[n - 1]))
    print(f"C{n:<2d} with mirror forms {c:6d} (known {A000628[n-1]:6d}) {'ok' if c == A000628[n-1]
else 'DIFF'}", flush=True)
print(f"exact: {sum(a == b for _, a, b in out)}/{len(out)}")
json.dump(out, open("stereo2.json", "w"))
```

# vaste_stof.py — metal line and coordination numbers

```
"""Solids: metal or not, and coordination numbers from the cube.
S1 (depth rule) An atom gives its outer passages away (metal) when they do not exceed its depth
   (the number of rings it stands on = period). Outer passages = s + p of the outermost shell.
   This equals Sanderson's rule.
S2 The cube offers exactly four neighbour sets: 4 alternate corners, 6 face centres,
   8 corners, 12 edge midpoints. Predicted coordination numbers of close-bound solids: 4, 6, 8, 12.
Data: mendeleev lattice_structure; metal/metalloid/nonmetal from the standard IUPAC-style list.
"""
import json, warnings; warnings.filterwarnings("ignore")
from mendeleev.fetch import fetch_table
el = fetch_table("elements").set_index("atomic_number")
nonmetal = set("H He C N O F Ne P S Cl Ar Se Br Kr I Xe Rn".split())
metalloid = set("B Si Ge As Sb Te".split())
ok = n = 0; miss = []
for Z in range(1, 87):
    sym = el.loc[Z, "symbol"]; per = int(el.loc[Z, "period"])
    ec = el.loc[Z, "electronic_configuration"]
    outer = sum(int(t[2:]) if len(t) > 2 else 1 for t in ec.split() if not t.startswith("[") and
t[1] in "sp" and int(t[0]) == per)
    pred_metal = outer <= per
    if sym in metalloid: continue                       # boundary: either answer accepted, not
counted
    real_metal = sym not in nonmetal
    n += 1; ok += pred_metal == real_metal
    if pred_metal != real_metal: miss.append(sym)
print(f"S1 metal / non-metal (Z<=86, metalloids left out): {ok}/{n}; misses {miss}")
# metalloids: on the boundary outer == per or outer == per+1?
mb = [(s, int(el[el.symbol == s].period.iloc[0])) for s in sorted(metalloid)]
print("metalloids (sym, period):", mb)
CN = {"BCC": 8, "FCC": 12, "HEX": 12, "DIA": 4, "SC": 6, "CUB": 6}
ls = el["lattice_structure"].dropna()
counts = {}
for Z, s in ls.items(): counts[s] = counts.get(s, 0) + 1
print("lattice types:", counts)
inset = sum(CN.get(s) in (4, 6, 8, 12) for s in ls.values)
print(f"S2 elements whose lattice has CN in {{4,6,8,12}}: {inset}/{len(ls)}")
json.dump({"S1": [ok, n, miss], "lattice": counts, "S2": [inset, len(ls)]}, open("vaste_stof.json",
"w"))
```

# fblok.py — lanthanide and actinide oxidation states

```
"""f-block repair. R2 says: a set with no inner ring of its kind (1s, 2p, 3d, 4f) is compact.
4f lies under the outer 5s 5p 6s rings and does not face outward. Rule F for the lanthanides:
the atom gives s2 plus one passage (+3); it gives one more f passage only when that brings the
f set to a closure (empty, or half = the ring of N3 at 7). 5f has an inner f ring and keeps rule A7.
Status: partly fitted (the 'one more to closure' clause was chosen after seeing Ce and Tb).
"""
import json
d = json.load(open("periodiek.json")); R = {r["sym"]: r for r in d["rows"]}
lan = "La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu".split()
act = "Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr".split()
def f_count(sym):
    return sum(int(t[2:]) for t in R[sym]["conf_pred"].split() if t[1:2] == "f" and len(t) > 2)
out = []; okL = okA = 0
for s in lan:
    k = f_count(s); left = k - 1 if k else 0        # after +3: s2 and one f (or d) passage gone
    pred = 3 + (1 if left in (1, 8) else 0)
    meas = R[s]["ox_max_meas"]; okL += pred == meas; out.append((s, k, pred, meas))
for s in act:
    pred = R[s]["ox_max_pred"]; meas = R[s]["ox_max_meas"]; okA += pred == meas; out.append((s,
f_count(s), pred, meas))
for o in out: print(o)
print(f"lanthanides rule F {okL}/15 (rule A7 gave {sum(R[s]['ox_max_pred']==R[s]['ox_max_meas'] for
s in lan)}/15); actinides rule A7 {okA}/15")
json.dump({"rows": out, "lan": okL, "act": okA}, open("fblok.json", "w"))
```

# chem_tree.py — shared tools: molecules as trees, mirror forms by rule G2

```
"""Shared tools: acyclic molecules as labelled trees, and counting their mirror forms.

Rules (from the book):
 M1  open passages: C 4, N 3, O 2, S 2, H 1. Hydrogens close what is left.
 M2  a bond is a meeting; a double bond is two meetings between the same pair.
 G2  a carbon with four single-bonded, pairwise different ligands takes one of the cube's two
     tetrahedra: a sign + or -. Ligands are compared *with* their signs, so mirror-image
     branches make a centre (pseudo-asymmetry). Mirror images of the whole molecule count apart.
Input: a small acyclic SMILES subset: atoms C N O S, bracket groups such as [Ph] (a ring
group treated as one ligand without centres), '=' for double bonds, '(' ')' for branches.
"""
import itertools, re
import networkx as nx

VAL = {"C": 4, "N": 3, "O": 2, "S": 2}

def parse(smiles):
    G = nx.Graph(); stack = []; prev = None; order = 1; i = 0; k = 0
    toks = re.findall(r"\[[^\]]+\]|[A-Z][a-z]?|=|\(|\)", smiles)
    for t in toks:
        if t == "(": stack.append(prev); continue
        if t == ")": prev = stack.pop(); continue
        if t == "=": order = 2; continue
        lab = t.strip("[]")
        G.add_node(k, el=lab)
        if prev is not None: G.add_edge(prev, k, order=order)
        prev = k; order = 1; k += 1
    return G

def hcount(G, v):
    el = G.nodes[v]["el"]
    if el not in VAL: return 0
    return VAL[el] - sum(G[v][u]["order"] for u in G[v])

def candidates(G):
    return [v for v in G if G.nodes[v]["el"] == "C" and all(G[v][u]["order"] == 1 for u in G[v])
            and hcount(G, v) <= 1 and G.degree(v) + hcount(G, v) == 4]

def _parity(perm):
    s, seen = 1, set()
    for i in range(len(perm)):
        if i in seen: continue
        j, L = i, 0
        while j not in seen: seen.add(j); j = perm[j]; L += 1
        if L % 2 == 0: s = -s
    return s

def _string(G, v, parent, sign):
    kids = sorted((("=" if G[v][c]["order"] == 2 else "") + _string(G, c, v, sign), c) for c in G[v]
if c != parent)
    nh = hcount(G, v)
    ligs = ([("P", parent)] if parent is not None else []) + list(kids) + [("H", None)] * nh
    desc = 0
    if v in sign and len(ligs) == 4 and len(set(l for l, _ in ligs)) == 4:
        raw = sorted(c for _, c in ligs if c is not None) + [None] * nh
        perm = [raw.index(c) for _, c in ligs]
        desc = sign[v] * _parity(perm)
    return G.nodes[v]["el"] + "(" + {1: "+", -1: "-", 0: ""}[desc] + "".join(s for s, _ in kids) +
")"

def canonical(G, sign=None):
    sign = sign or {}
    return min(_string(G, r, None, sign) for r in nx.center(G))

def stereo_forms(G):
    """Number of distinct molecules (mirror images counted apart) and the stereogenic centres."""
    cand = candidates(G)
    forms = set()
    for signs in itertools.product((1, -1), repeat=len(cand)):
        forms.add(canonical(G, dict(zip(cand, signs))))
    centres = [v for v in cand if any(
        canonical(G, {v: 1}) != canonical(G, {v: -1}) or True for _ in [0])]
    return len(forms)

def chiral(G):
    """True if some signed form differs from its mirror image."""
    cand = candidates(G)
    for signs in itertools.product((1, -1), repeat=len(cand)):
        a = canonical(G, dict(zip(cand, signs)))
        b = canonical(G, dict(zip(cand, [-s for s in signs])))
        if a != b: return True
    return False
```

# organisch.py — alcohols, rings and double bonds, benzene isomers, oxyacids

```
"""Organic chemistry from the closure rule.
O1 Alcohols C_nH_(2n+1)OH: every closed carbon tree with one OH; with and without mirror forms.
   Known: OEIS A000598 and A000625 (alkyl groups; one alkyl group per alcohol).
O2 Degree of unsaturation from passage counting: P open passages, N atoms. A connected molecule
   needs N-1 meetings (2(N-1) passages); the rest pair into rings or extra bonds:
   DoU = (P - 2(N - 1)) / 2 = (2C + 2 + N - H - X) / 2.
O3 Substituted benzene: the hexagon of the cube, with its 12 symmetries (6 turns, 6 flips).
O4 Oxyacids: the leftover passage of the anion is shared over the equivalent oxygens.
   More sharing places -> stronger acid. Places = p + 1 (p = oxygens without H).
"""
import itertools, json
import networkx as nx
from chem_tree import canonical, stereo_forms

A000598 = [1, 1, 2, 4, 8, 17, 39, 89, 211, 507]
A000625 = [1, 1, 2, 5, 11, 28, 74, 199, 551, 1553]
out = {"O1": []}
for n in range(1, 11):
    trees = [nx.empty_graph(1)] if n == 1 else [T for T in nx.nonisomorphic_trees(n) if
max(dict(T.degree()).values()) <= 4]
    cons = {}
    for T in trees:
        for v in T:
            if T.degree(v) > 3: continue
            G = nx.Graph()
            for u in T: G.add_node(u, el="C")
            for a, b in T.edges(): G.add_edge(a, b, order=1)
            G.add_node(n, el="O"); G.add_edge(v, n, order=1)
            cons.setdefault(canonical(G), G)
    st = sum(stereo_forms(G) for G in cons.values())
    out["O1"].append((n, len(cons), A000598[n - 1], st, A000625[n - 1]))
    print(f"C{n}H{2*n+1}OH  alcohols {len(cons):5d} (known {A000598[n-1]:5d})  with mirror forms
{st:5d} (known {A000625[n-1]:5d})", flush=True)

# O2
VAL = {"C": 4, "H": 1, "N": 3, "O": 2, "F": 1, "Cl": 1, "Br": 1}
tests = {  # formula: known rings + pi bonds
 "C6H6 benzene": ({"C": 6, "H": 6}, 4), "C2H4 ethene": ({"C": 2, "H": 4}, 1), "C2H2 ethyne": ({"C":
2, "H": 2}, 2),
 "C6H12 cyclohexane": ({"C": 6, "H": 12}, 1), "C10H8 naphthalene": ({"C": 10, "H": 8}, 7), "C5H5N
pyridine": ({"C": 5, "H": 5, "N": 1}, 4),
 "C6H12O6 glucose (open)": ({"C": 6, "H": 12, "O": 6}, 1), "C8H10N4O2 caffeine": ({"C": 8, "H": 10,
"N": 4, "O": 2}, 6),
 "C9H8O4 aspirin": ({"C": 9, "H": 8, "O": 4}, 6), "C20H25N3O LSD": ({"C": 20, "H": 25, "N": 3, "O":
1}, 10),
 "C27H46O cholesterol": ({"C": 27, "H": 46, "O": 1}, 5), "C60 fullerene (31 independent rings + 30
double bonds)": ({"C": 60}, 61),
 "CHCl3 chloroform": ({"C": 1, "H": 1, "Cl": 3}, 0), "C6H5Br bromobenzene": ({"C": 6, "H": 5, "Br":
1}, 4),
}
o2 = []
for name, (f, known) in tests.items():
    Pp = sum(VAL[e] * k for e, k in f.items()); N = sum(f.values())
    dou = (Pp - 2 * (N - 1)) // 2
    o2.append((name, dou, known, dou == known))
    print(f"O2 {name:28s} DoU {dou:3d} known {known:3d}")
out["O2"] = o2

# O3 benzene substitution patterns under the 12 symmetries of the hexagon
rot = [tuple((i + r) % 6 for i in range(6)) for r in range(6)]
flip = [tuple((r - i) % 6 for i in range(6)) for r in range(6)]
G12 = rot + flip
def patterns(multiset):
    seen = set()
    for perm in set(itertools.permutations(multiset)):
        seen.add(min(tuple(perm[g[i]] for i in range(6)) for g in G12))
    return len(seen)
cases = [("C6H5X", "HHHHHX", 1), ("C6H4X2", "HHHHXX", 3), ("C6H4XY", "HHHHXY", 3), ("C6H3X3",
"HHHXXX", 3),
         ("C6H3X2Y", "HHHXXY", 6), ("C6H3XYZ", "HHHXYZ", 10), ("C6H2X4", "HHXXXX", 3), ("C6HX5",
"HXXXXX", 1), ("C6X6", "XXXXXX", 1)]
o3 = []
for f, m, known in cases:
    c = patterns(m); o3.append((f, c, known, c == known)); print(f"O3 {f:8s} isomers {c:3d} known
{known:3d}")
out["O3"] = o3

# O4 oxyacids: (name, oxygens without H = p, pKa1 measured)
acids = [("HClO", 0, 7.53), ("HBrO", 0, 8.6), ("HIO", 0, 10.6), ("H3BO3", 0, 9.24), ("H4SiO4", 0,
9.8),
         ("H3AsO3", 0, 9.2), ("HClO2", 1, 1.96), ("HNO2", 1, 3.35), ("H3PO4", 1, 2.15), ("H3AsO4",
1, 2.19),
```

```
        ("H2SO3", 1, 1.86), ("H2SeO3", 1, 2.62), ("HIO3", 2, 0.77), ("HClO3", 2, -1.0), ("HNO3", 2,
-1.4),
        ("H2SO4", 2, -3.0), ("H2SeO4", 2, -2.0), ("HClO4", 3, -10.0), ("HMnO4", 3, -2.2)]
import statistics
def ranks(x):
    s = sorted(range(len(x)), key=lambda i: x[i]); r = [0] * len(x)
    i = 0
    while i < len(s):
        j = i
        while j + 1 < len(s) and x[s[j + 1]] == x[s[i]]: j += 1
        for k in range(i, j + 1): r[s[k]] = (i + j) / 2
        i = j + 1
    return r
pl = [a[1] + 1 for a in acids]; pk = [a[2] for a in acids]
rp, rk = ranks(pl), ranks(pk)
mx, my = statistics.mean(rp), statistics.mean(rk)
rho = sum((a - mx) * (b - my) for a, b in zip(rp, rk)) / (sum((a - mx) ** 2 for a in rp) * sum((b -
my) ** 2 for b in rk)) ** 0.5
for pv in range(4):
    vals = [a[2] for a in acids if a[1] == pv]
    print(f"O4 places {pv+1}: n={len(vals)} mean pKa {statistics.mean(vals):.2f}  (Pauling 8-5p:
{8-5*pv})")
print(f"O4 Spearman rank correlation, places vs pKa: {rho:.3f}")
out["O4"] = {"acids": acids, "rho": rho, "means": [round(statistics.mean([a[2] for a in acids if
a[1] == pv]), 2) for pv in range(4)]}
json.dump(out, open("organisch.json", "w"))
```

# biochemie.py — sugars, polyols, hydroxy acids, amino acids, base pairs, genetic code

```
"""Biochemistry from the closure rule.
B1 Sugars, sugar alcohols, hydroxy acids, amino acids: number of forms (mirror images apart),
   counted with chem_tree (rule G2, including pseudo-asymmetric centres). Known values: textbooks.
B2 Base pairing. Each base edge is a word of three places: donor +1, acceptor -1, nothing 0.
   A pair forms where the words meet (x, -x) without a clash (x, x), and where the ring count of
   the pair is three: a window of three (purine 2 rings + pyrimidine 1 ring).
B3 The genetic code read as windows of three: how often a change at each place keeps the amino acid.
"""
import itertools, json
from chem_tree import parse, stereo_forms

MOLS = [  # name, acyclic SMILES (subset), known number of forms incl. mirror images, class
 ("glycerol", "OCC(O)CO", 1, "polyol"),
 ("glyceraldehyde", "OCC(O)C=O", 2, "sugar"),
 ("aldotetroses", "OCC(O)C(O)C=O", 4, "sugar"),
 ("aldopentoses", "OCC(O)C(O)C(O)C=O", 8, "sugar"),
 ("aldohexoses", "OCC(O)C(O)C(O)C(O)C=O", 16, "sugar"),
 ("ketotriose (dihydroxyacetone)", "OCC(=O)CO", 1, "sugar"),
 ("ketotetroses", "OCC(=O)C(O)CO", 2, "sugar"),
 ("ketopentoses", "OCC(=O)C(O)C(O)CO", 4, "sugar"),
 ("ketohexoses", "OCC(=O)C(O)C(O)C(O)CO", 8, "sugar"),
 ("tetritols (erythritol, threitol)", "OCC(O)C(O)CO", 3, "polyol"),
 ("pentitols (ribitol, xylitol, arabitol)", "OCC(O)C(O)C(O)CO", 4, "polyol"),
 ("hexitols (sorbitol, mannitol, …)", "OCC(O)C(O)C(O)C(O)CO", 10, "polyol"),
 ("tartaric acid", "OC(=O)C(O)C(O)C(=O)O", 3, "acid"),
 ("lactic acid", "CC(O)C(=O)O", 2, "acid"),
 ("malic acid", "OC(=O)CC(O)C(=O)O", 2, "acid"),
 ("citric acid", "OC(=O)CC(O)(CC(=O)O)C(=O)O", 1, "acid"),
 ("trihydroxyglutaric acid", "OC(=O)C(O)C(O)C(O)C(=O)O", 4, "acid"),
 ("glycine", "NCC(=O)O", 1, "amino acid"),
 ("alanine", "NC(C)C(=O)O", 2, "amino acid"),
 ("valine", "NC(C(C)C)C(=O)O", 2, "amino acid"),
 ("leucine", "NC(CC(C)C)C(=O)O", 2, "amino acid"),
 ("isoleucine", "NC(C(C)CC)C(=O)O", 4, "amino acid"),
 ("serine", "NC(CO)C(=O)O", 2, "amino acid"),
 ("threonine", "NC(C(C)O)C(=O)O", 4, "amino acid"),
 ("cysteine", "NC(CS)C(=O)O", 2, "amino acid"),
 ("methionine", "NC(CCSC)C(=O)O", 2, "amino acid"),
 ("aspartic acid", "NC(CC(=O)O)C(=O)O", 2, "amino acid"),
 ("glutamic acid", "NC(CCC(=O)O)C(=O)O", 2, "amino acid"),
 ("asparagine", "NC(CC(=O)N)C(=O)O", 2, "amino acid"),
 ("glutamine", "NC(CCC(=O)N)C(=O)O", 2, "amino acid"),
 ("lysine", "NC(CCCCN)C(=O)O", 2, "amino acid"),
 ("arginine", "NC(CCCNC(=N)N)C(=O)O", 2, "amino acid"),
 ("phenylalanine", "NC(C[Ph])C(=O)O", 2, "amino acid"),
 ("tyrosine", "NC(C[HOPh])C(=O)O", 2, "amino acid"),
 ("tryptophan", "NC(C[Indolyl])C(=O)O", 2, "amino acid"),
 ("histidine", "NC(C[Imidazolyl])C(=O)O", 2, "amino acid"),
]
res = []
for name, smi, known, cls in MOLS:
    n = stereo_forms(parse(smi))
    res.append((name, cls, n, known, n == known))
```

```
    print(f"{name:40s} {n:3d}  known {known:3d}  {'ok' if n == known else 'DIFF'}")
print(f"B1: {sum(r[4] for r in res)}/{len(res)} exact (proline, a ring, checked separately with
RDKit)")
try:
    from rdkit import Chem
    pro = Chem.MolFromSmiles("OC(=O)C1CCCN1")
    print("proline stereocentres (RDKit):", Chem.FindMolChiralCenters(pro, includeUnassigned=True))
except Exception as e:
    print("rdkit check skipped", e)

# B2 base pairing
W = {"A": ((+1, -1, 0), 2), "G": ((-1, +1, +1), 2), "C": ((+1, -1, -1), 1), "T": ((-1, +1, -1), 1)}
pairs = []
for x, y in itertools.combinations_with_replacement("ACGT", 2):
    (wx, rx), (wy, ry) = W[x], W[y]
    meet = sum(1 for a, b in zip(wx, wy) if a and b and a == -b)
    clash = sum(1 for a, b in zip(wx, wy) if a and a == b)
    width_ok = rx + ry == 3
    forms = width_ok and clash == 0 and meet >= 2
    real = {x, y} in ({"A", "T"}, {"C", "G"})
    pairs.append((x + "·" + y, meet, clash, rx + ry, forms, real))
    print(f"{x}·{y}: meetings {meet}, clashes {clash}, rings {rx+ry} -> pair {forms}  (Watson-Crick
{real})")
print("B2 right:", sum(p[4] == p[5] for p in pairs), "/", len(pairs))
print("G = -C exactly:", tuple(-v for v in W["C"][0]) == W["G"][0], "; T vs -A:", W["T"][0], tuple(-
v for v in W["A"][0]))

# B3 genetic code (standard table)
bases = "TCAG"
aa = "FFLLSSSSYY**CC*WLLLLPPPPHHQQRRRRIIIMTTTTNNKKSSRRVVVVAAAADDEEGGGG"
code = {a + b + c: aa[16 * i + 4 * j + k] for i, a in enumerate(bases) for j, b in enumerate(bases)
for k, c in enumerate(bases)}
syn = [0, 0, 0]; tot = [0, 0, 0]
for cod, a in code.items():
    if a == "*": continue
    for p in range(3):
        for b in bases:
            if b == cod[p]: continue
            m = cod[:p] + b + cod[p + 1:]
            if code[m] == "*": continue
            tot[p] += 1; syn[p] += code[m] == a
frac = [round(s / t, 3) for s, t in zip(syn, tot)]
print("B3 synonymous fraction by place 1,2,3:", frac, "; amino acids:", len(set(aa) - {"*"}), ";
sense codons:", sum(a != "*" for a in code.values()))
json.dump({"B1": res, "B2": pairs, "B3": frac}, open("biochemie.json", "w"))
```

# biofysica.py — ice rule, residual entropy, square ice

```
"""Biophysics from the closure rule: water, ice and the hydrogen bond.
F1 A hydrogen bond is a meeting: donor +1 against acceptor -1.
   Water has two donors and two acceptors: its word (+1, +1, -1, -1) sums to zero.
   Each water closes with four neighbours: coordination 4 (the cube's alternate corners), two
   hydrogen bonds per molecule.
F2 Ice rule = closure rule. On every oxygen the four bond values (+1 hydrogen near, -1 far)
   must sum to zero. Of the 16 words of length 4, C(4,2) = 6 close.
   Pauling count: W = 2^(2N) (6/16)^N = (3/2)^N, so S = R ln(3/2).
F3 Exact check of the closure count on the square lattice (square ice), by transfer matrix,
   against Lieb's exact result W = (4/3)^(3/2) = 1.5396.
"""
import itertools, json, math
import numpy as np
R = 8.314462618
closing = [w for w in itertools.product((1, -1), repeat=4) if sum(w) == 0]
W_pauling = 4 * len(closing) / 16
S_pauling = R * math.log(W_pauling)
S_meas, S_err = 3.41, 0.2     # Giauque & Stout 1936
W_nagle = 1.50685             # Nagle 1966, exact series for ice Ih
print(f"F2 closing words {len(closing)}/16; W = {W_pauling}; S = R ln W = {S_pauling:.3f} J/(mol K);
measured {S_meas} ± {S_err}; Nagle {R*math.log(W_nagle):.3f}")

def transfer(L):
    states = list(itertools.product((1, -1), repeat=L))
    T = np.zeros((len(states), len(states)))
    for a, v in enumerate(states):
        for b, u in enumerate(states):
            c = 0
            for h0 in (1, -1):
                h = h0; ok = True
                for i in range(L):
                    h = h + v[i] - u[i]
                    if h not in (1, -1): ok = False; break
                if ok and h == h0: c += 1
            T[a, b] = c
    return T
```

```
lieb = (4 / 3) ** 1.5
f3 = []
for L in (2, 4, 6, 8, 10):
    lam = max(abs(np.linalg.eigvals(transfer(L))))
    w = lam ** (1 / L)
    f3.append((L, round(float(w), 5)))
    print(f"F3 square ice, strip width {L:2d}: W per site {w:.5f}   (Lieb exact {lieb:.5f}, mean-
field closure 1.5)", flush=True)
json.dump({"F2": {"W": W_pauling, "S": S_pauling, "S_meas": S_meas, "S_err": S_err, "S_nagle": R *
math.log(W_nagle)},
           "F3": f3, "lieb": lieb}, open("biofysica.json", "w"))
# extrapolation w(L) = w_inf + a / L^2 from the two widest strips
(L1, w1), (L2, w2) = f3[-2], f3[-1]
w_inf = (L2 ** 2 * w2 - L1 ** 2 * w1) / (L2 ** 2 - L1 ** 2)
print(f"F3 extrapolated W per site {w_inf:.5f}  (Lieb {lieb:.5f}; difference {abs(w_inf -
lieb):.5f})")
d = json.load(open("biofysica.json")); d["F3_extrap"] = w_inf; json.dump(d, open("biofysica.json",
"w"))
```

# spectra.py — hydrogen line ratios and one-electron ions

```
"""Light from the atom.
L1 (reading) A shell of depth n has n^2 places (half its capacity 2n^2). One closure binds the
   shell; it is shared over its n^2 places. So the binding per passage goes as 1/n^2.
L2 (reading) A centre that carries Z passages binds a single passage Z times as strongly at
   Z times smaller depth scale: Z^2.
Then a jump n2 -> n1 gives light with 1/lambda proportional to Z^2 (1/n1^2 - 1/n2^2).
Unit-free tests: wavelength ratios inside a series (Wikipedia: Lyman vacuum, Balmer and Paschen air)
and ionisation energies of one-electron ions divided by that of hydrogen (NIST via mendeleev).
"""
import json, warnings; warnings.filterwarnings("ignore")
from mendeleev.fetch import fetch_table
series = {"Lyman": (1, {2: 121.57, 3: 102.57, 4: 97.254, 5: 94.974}),
          "Balmer": (2, {3: 656.3, 4: 486.1, 5: 434.0, 6: 410.2}),
          "Paschen": (3, {4: 1875, 5: 1282, 6: 1094})}
rows = []
for name, (n1, lines) in series.items():
    first = min(lines)
    for n2, lam in lines.items():
        if n2 == first: continue
        pred = (1 / n1**2 - 1 / first**2) / (1 / n1**2 - 1 / n2**2)   # lambda(n2)/lambda(first)
        meas = lam / lines[first]
        rows.append((name, f"{n2}→{n1} / {first}→{n1}", round(pred, 5), round(meas, 5), round((meas
- pred) / pred * 100, 3)))
        print(rows[-1])
ie = fetch_table("ionizationenergies")
H = float(ie[(ie.atomic_number == 1) & (ie.ion_charge == 0)].ionization_energy.iloc[0])
zrows = []
for Z in range(1, 11):
    sel = ie[(ie.atomic_number == Z) & (ie.ion_charge == Z - 1)]
    if sel.empty: continue
    e = float(sel.ionization_energy.iloc[0])
    zrows.append((Z, round(e, 3), round(e / H, 4), Z * Z, round((e / H - Z * Z) / (Z * Z) * 100,
3)))
    print("Z", zrows[-1])
json.dump({"lines": rows, "Z2": zrows}, open("spectra.json", "w"))
```

# Annotated References


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*Why read it:* The n + l filling rule. Part II gives it a cost reading.

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*Why read it:* The logarithmic bond-order law, derived in Part III from depth.

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*Why read it:* The 4n + 2 rule, shown in Part V to be the atomic count again.

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