P0-A2 Ionization Energy Sawtooth (Mathematical Derivation + NIST Validation Tables)

Recognition Science Derivation Campaign

2026-01-17

Abstract

This document rewrites the P0-A2 ionization "sawtooth" result as a full mathematical derivation. The repository's Lean scaffold defines an *ionization proxy* $P(Z)$ from the period boundary maps and proves that, within each period, $P(Z)$ increases from the first element (alkali) to the closure endpoint (noble gas), and then resets after each closure. We then reproduce the preregistered validator tables comparing these ordering predictions to NIST first ionization energies (PASS 3/3 hard tests).

1 Claim (P0-A2)

Let $I_1(Z)$ denote the first ionization energy (in eV) for atomic number Z. Empirically, I_1 exhibits a characteristic sawtooth pattern across periods. In this repository, the fit-free content is an **ordering prediction**:

- Within each period, the ionization proxy increases from the alkali metal to the noble gas.
- Across a period boundary, the proxy resets downward at the next alkali.

The validator compares these ordering predictions to NIST data for $Z \leq 86$.

2 Definitions

We reuse the closure maps $\mathrm{prev}(Z)$ and $\mathrm{next}(Z)$ from P0-A0. Define the derived period length and valence position

$$\mathrm{periodLen}(Z) := \mathrm{next}(Z) - \mathrm{prev}(Z), \qquad \mathrm{valence}(Z) := Z - \mathrm{prev}(Z).$$

Definition 1 (Ionization proxy)**.** *Define the ionization proxy by*

$$P(Z) := \mathrm{valence}(Z).$$

In the Lean file this is `ionizationProxy Z := valenceElectrons Z`*.*

Definition 2 (Normalized and ϕ-scaled display seams)**.** *The implementation also defines (for display) a normalized value*

$$\mathrm{norm}(Z) := \begin{cases} 0 & \mathrm{periodLen}(Z) = 0, \\ \frac{P(Z)}{\mathrm{periodLen}(Z)} & \mathrm{periodLen}(Z) > 0, \end{cases}$$

and a ϕ-scaled quantity $\mathrm{scaled}(Z) = \phi^{2 \cdot \mathrm{period}(Z)} \cdot \mathrm{norm}(Z)$*. The ordering theorems below are proved at the proxy level $P(Z)$ (fit-free).*

3 Derivations (proxy-level ordering)

3.1 Alkali metals have minimal proxy within a period

Proposition 1. *If Z is the first element after a closure, i.e. $Z = \mathrm{prev}(Z) + 1$, then $P(Z) = 1$.*

Proof. By definition,

$$P(Z) = Z - \mathrm{prev}(Z) = (\mathrm{prev}(Z) + 1) - \mathrm{prev}(Z) = 1.$$

□

3.2 Noble gases have maximal proxy within a period

Proposition 2. *If Z is a closure endpoint (a noble gas in the chemistry scaffold), i.e. $\mathrm{next}(Z) = Z$, then*

$$P(Z) = \mathrm{periodLen}(Z).$$

Proof. If $\mathrm{next}(Z) = Z$, then

$$\mathrm{periodLen}(Z) = \mathrm{next}(Z) - \mathrm{prev}(Z) = Z - \mathrm{prev}(Z) = P(Z).$$

□

3.3 Monotonicity within a fixed period

Theorem 1. *If $Z_1 < Z_2$ and $\mathrm{prev}(Z_1) = \mathrm{prev}(Z_2)$ (so no boundary is crossed), then $P(Z_1) < P(Z_2)$.*

Proof. Let $c := \mathrm{prev}(Z_1) = \mathrm{prev}(Z_2)$. Then

$$P(Z_1) = Z_1 - c < Z_2 - c = P(Z_2).$$

□

3.4 Sawtooth reset across a boundary

Theorem 2. *If Z_{noble} is a closure endpoint and $Z_{\mathrm{alkali}} = Z_{\mathrm{noble}} + 1$, then*

$$P(Z_{\mathrm{alkali}}) < P(Z_{\mathrm{noble}}).$$

Proof. Because Z_{alkali} is the first element of the next period, $\mathrm{prev}(Z_{\mathrm{alkali}}) = Z_{\mathrm{noble}}$. Hence $P(Z_{\mathrm{alkali}}) = 1$ by the first proposition. Meanwhile $P(Z_{\mathrm{noble}}) = \mathrm{periodLen}(Z_{\mathrm{noble}})$ by the previous proposition, and in the scaffold $\mathrm{periodLen}(Z_{\mathrm{noble}}) \geq 2$, so $1 < P(Z_{\mathrm{noble}})$. □

4 Validation against NIST first ionization energies

The preregistered validator `scripts/analysis/chem_ionization_energy_compare.py` writes `artifacts/chem_ionization_energy_comparison.json`. The committed artifact reports **PASS (3/3 hard tests)** for $Z \leq 86$.

4.1 Hard test 1: alkali minimum within period (main group)

Alkali Z	Element	I_1 (eV)	Period	Pass
3	Li	5.392	3–10	true
11	Na	5.139	11–18	true
19	K	4.341	19–36	true
37	Rb	4.177	37–54	true
55	Cs	3.894	55–86	true

4.2 Hard test 2: noble maximum within period

Noble Z	Element	I_1 (eV)	Period	Pass
2	He	24.587	1–2	true
10	Ne	21.565	3–10	true
18	Ar	15.760	11–18	true
36	Kr	14.000	19–36	true
54	Xe	12.130	37–54	true
86	Rn	10.749	55–86	true

4.3 Hard test 3: sawtooth reset across boundary

Alkali Z	Element	I_1 (eV)	Prev. noble Z	Element	I_1 (eV)	Pass
3	Li	5.392	2	He	24.587	true
11	Na	5.139	10	Ne	21.565	true
19	K	4.341	18	Ar	15.760	true
37	Rb	4.177	36	Kr	14.000	true
55	Cs	3.894	54	Xe	12.130	true

4.4 Note on "proxy ordering" violations

The validator additionally counts local anomalies where the strictly increasing proxy does not match strict increase in the NIST values (e.g. Be $\to$ B, N $\to$ O). These are recorded as informational and are not treated as a hard falsifier in the current prereg.

5 Repo cross-references

Lean modules:

- `IndisputableMonolith/Chemistry/IonizationEnergy.lean`
- `IndisputableMonolith/Chemistry/PeriodicTable.lean` (period/valence primitives)

Key proved theorems (names as exported in the module):

- `alkali_min_ionization`: if `valenceElectrons Z = 1` then `ionizationProxy Z = 1`
- `noble_max_ionization`: if `isNobleGas Z` then `ionizationProxy Z = periodLength Z`
- `ionization_monotone_within_period`: same-period implies strict increase in proxy
- `sawtooth_reset`: if `Zalkali = Znoble + 1` then `proxy(Zalkali) < proxy(Znoble)`

Artifact reference. Validation output: artifacts/chem_ionization_energy_comparison.json.