

Supplementary Information

Exchange-counting support for the Madelung anomaly ladder

Associated manuscript: Explaining the Madelung Anomalies: From Chemical Slogans to an Exchange-Counting Ladder

Author: Maisara Shoeib

S1. Purpose

This supplement documents the reproducibility materials for the Madelung anomaly ladder paper. It regenerates the exchange-counting tables, signed-threshold table, exchange-coefficient checks, and final figures used in the manuscript. It is deliberately compact: it is an audit trail for the arithmetic and figures, not a hidden predictor and not the full WIM selector project.

S2. Reproduction command

Run from the package root: `pip install -r requirements.txt`, then `python run_all.py`. Optional tests can be executed with `pytest -q`. The scripts write regenerated figures to `figures/` and regenerated CSV/log files to `outputs/`.

S3. Leakage-control statement

The scripts do not read an adopted configuration-label table. The Tier I and f/d tables are generated from explicitly stated cases and equations. Fixed empirical level values are used only for magnitude discussion and are not used to derive the exchange-counting rules.

S4. Boundary of the claim

The supplement supports the paper's bounded claim: eight sd cases have an exact exchange-counting skeleton; five cases are mechanism-supported but magnitude-open; seven early f/d cases require self-consistent relativistic and multiconfiguration input. The code does not replace ab initio atomic-structure calculations and does not compute absolute many-electron energies.

S5. Package structure

Path	Role
scripts/derive_exchange.py	Derives Kbar coefficients by Wigner-3j summation and checks the d5 6S Condon-Shortley anchor.
scripts/generate_figures.py	Regenerates Table 1, Table 2, empirical magnitude targets, and Figures 1-4.
figures/	Final PNG figure files used by the manuscript.
outputs/	Regenerated CSV tables, logs, environment record, and checksums.
tests/	Lightweight reproducibility tests.
run_all.py	One-command wrapper for the reproduction scripts.

S6. Expected exact checks

Quantity	Expected result
Kbar_dd	$(2/35) F_2 + (4/63) F_4$
Kbar_ff	$(8/225) F_2 + (8/297) F_4 + (200/5577) F_6$
d5 6S check, k=2	$-35 * F_2$
d5 6S check, k=4	$-315 * F_4$
Non-case check	$dX(d5 \rightarrow d6) = 0; dX_f(7 \rightarrow 8) = 0$

S7. Generated files

The generated tables are outputs/table1_tier1_sd_pair_counts.csv, outputs/table2_fd_signed_thresholds.csv, outputs/empirical_magnitude_targets.csv, outputs/exchange_coefficients_summary.csv, outputs/exchange_sixS_condon_shortley_check.csv, and outputs/indicative_exchange_scales.csv. The generated figures are figures/fig1_ladder.png, figures/fig2_deltaX_revised_clean.png, figures/fig3_thresholds.png, and figures/fig4_veff.png.

End of supplementary information.