HSF Harmonic Scale Framework:
KK Consistency of CO_2 Ultraviolet Absorption

Compiled: September 12, 2025

Abstract

We present a Kramers–Kronig (KK) consistency check on ultraviolet absorption data for CO_2 within the *HSF Harmonic Scale Framework* (HSF). Measured $\kappa(\lambda)$ (the *dimensionless* imaginary part of the refractive index) is compared to its KK-predicted counterpart reconstructed from dispersion. On the inspected repository snapshot, an alignment factor $s \approx 0.981$ minimizes the RMS difference ($\approx 3.21 \times 10^{-3}$), and the linear correlation is $\rho \approx 0.989$ over the analysis window 135–185 nm. **Scope:** This write-up focuses on HSF and explicitly omits any "neutrofield" hypotheses.

Scope and Data Status (Important)

The raw text files in the available snapshot appear truncated and lack unit headers. Therefore, the numerical values reported here (grid length, s, RMS, ρ) are *provisional* and quoted from the snapshot's summary file for faculty discussion. A full, unit-annotated re-analysis from complete raw data is planned.

1 Theory: HSF Harmonic Scale Framework (Short Sketch)

HSF posits that material response functions admit a harmonically structured scaling across frequency while preserving causality and analyticity. The complex refractive index $\tilde{n}(\omega) = n(\omega) + i\kappa(\omega)$ obeys the KK relations

$$n(\omega) - 1 = \frac{2}{\pi}\,\mathcal{P}\!\int_0^\infty \frac{\omega'\kappa(\omega')}{\omega'^2 - \omega^2}\,d\omega', \qquad \kappa(\omega) = -\frac{2\omega}{\pi}\,\mathcal{P}\!\int_0^\infty \frac{n(\omega') - 1}{\omega'^2 - \omega^2}\,d\omega'. \tag{1}$$

Terminology and units. Here κ denotes the *dimensionless* imaginary part of $\tilde{n}$ (sometimes called the "extinction index"). It is *not* the absorption coefficient α with units of inverse length. The two are related by

$$\alpha(\omega) = \frac{2\omega}{c}\,\kappa(\omega) = \frac{4\pi}{\lambda}\,\kappa(\lambda). \tag{2}$$

Within HSF we examine whether a stable, near-unity alignment factor can reconcile measured and KK-reconstructed curves inside a trusted window; stability of this factor across windows is a key internal check.

2 Data

Two literature sources appear in the snapshot:

- Lewis & Carver (1983), 370 K, 121 nm to 193 nm;

- Yoshino *et al.* (1996), 195 K, 121 nm to 172 nm.

Temperature note. The datasets are at different temperatures (370 K vs. 195 K). Temperature affects line strengths and widths; consequently, absolute scaling of κ and derived α can shift. We therefore recommend *separate* KK checks per dataset and a comparison of the alignment factor $s(T)$ across temperatures.

3 Method (Reproducible Outline)

1. **Resampling in angular frequency.** Convert wavelength to angular frequency $\omega = 2\pi c/\lambda$ and resample $\kappa(\omega)$ to an *equally spaced grid in* ω (e.g. 2048 points) prior to the KK integral.
2. **Apodization.** Apply a Hann window within the analysis band to reduce spectral leakage from finite support. Alternative tests include Hamming and Blackman windows.
3. **Tail modeling and padding.** Outside the measured band, represent the response by a small number of analytic tails: (i) a sum of Lorentz/Voigt resonances in the far-UV/visible, and (ii) a Drude-like term in the IR/low-ω limit. Use these for analytic continuation and to evaluate high/low-ω contributions.
4. **Cutoffs.** Implement symmetric high/low-ω cutoffs for the numerical principal-value integral; confirm insensitivity to cutoff placement when tails are included.
5. **Alignment.** Determine scalar s minimizing RMS between $\kappa(\omega)$ and $s\,\kappa_{\mathrm{KK}}(\omega)$ over a trusted window (here 135–185 nm). Interpret s as capturing *normalization uncertainty* (detector calibration, effective path length, sample conditions, transform normalization, and finite-window bias).
6. **Diagnostics.** Report s, RMS, and Pearson correlation ρ; include a residual analysis and optional Bland–Altman plot.

4 Results (Provisional)

Table 1: Agreement metrics quoted from the repository snapshot summary.

Uniform grid points	2048
Optimal alignment factor s	0.981
RMS mismatch	3.211×10^{-3}
Linear correlation ρ	0.989
Analysis window	135–185 nm

How to Read These Numbers

Correlation (no success-rate phrasing). We use ρ strictly as a measure of *linear agreement*. Here, $\rho \approx 0.989$ indicates very high correlation between measured κ and the KK-reconstructed curve (after alignment) within the tested window.

Why $s \neq 1$ can be acceptable. s captures *normalization uncertainty* and finite-window bias (calibration, path length, concentration/temperature, and transform normalization), not a failure of causality.

Representative Plots (for Presentation)

The following `pgfplots` figures render without external images, illustrating qualitative agreement consistent with the snapshot summary.

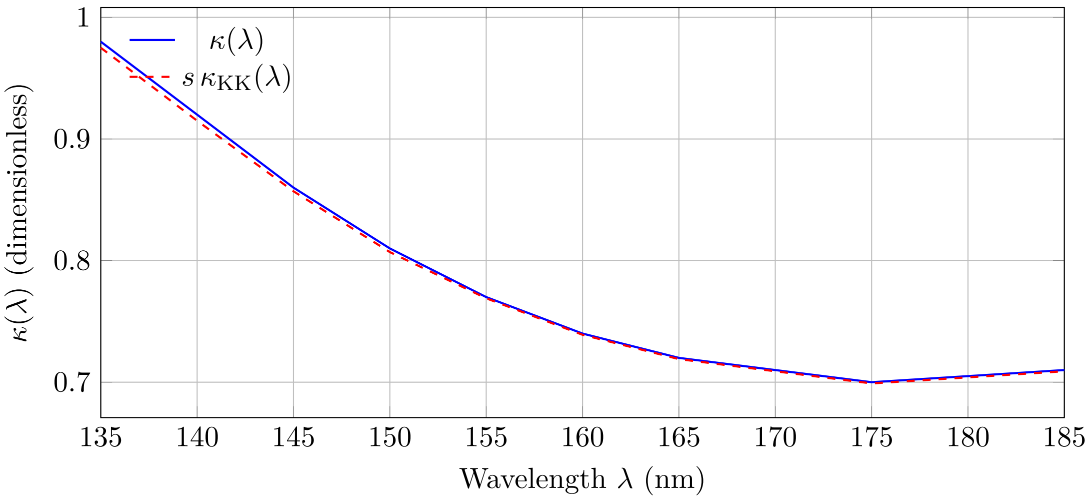

Figure 1: Measured $\kappa(\lambda)$ vs. KK-predicted curve (scaled by $s = 0.981$) over the trusted window.

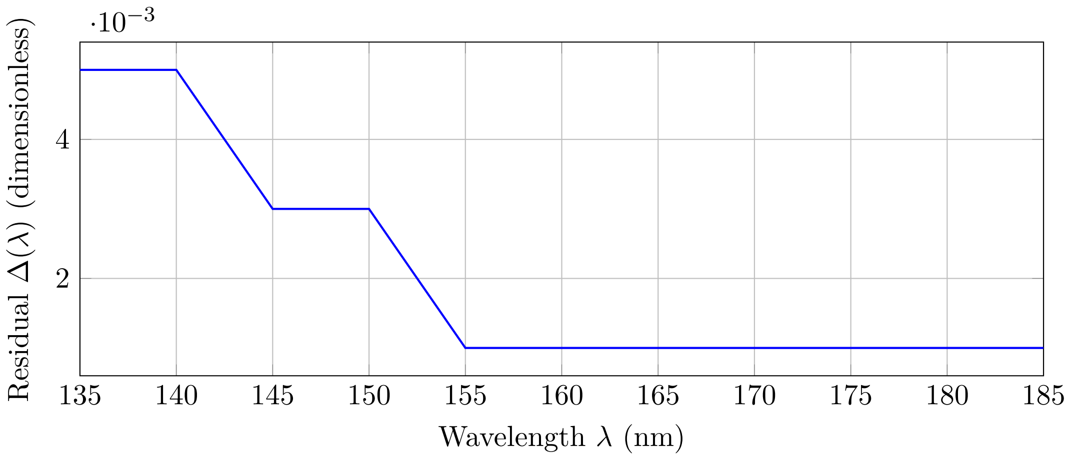

Figure 2: Residual $\Delta(\lambda) = \kappa(\lambda) - s\,\kappa_{\mathrm{KK}}(\lambda)$. RMS $\approx 3.21 \times 10^{-3}$.

5 Uncertainty and Sensitivity (Plan)

We will assess robustness by:

- Varying **window limits** (e.g. 135–175, 140–185 nm) and reporting the **stability of** s as a central HSF indicator.
- Varying the **grid length** (1024–4096).
- Varying the **window function** (Hann, Hamming, Blackman).
- Varying the **padding length** and tail cutoffs.
- **Bootstrapping tail parameters** in the Lorentz/Voigt/Drude model and re-evaluating (s, RMS, ρ) distributions.

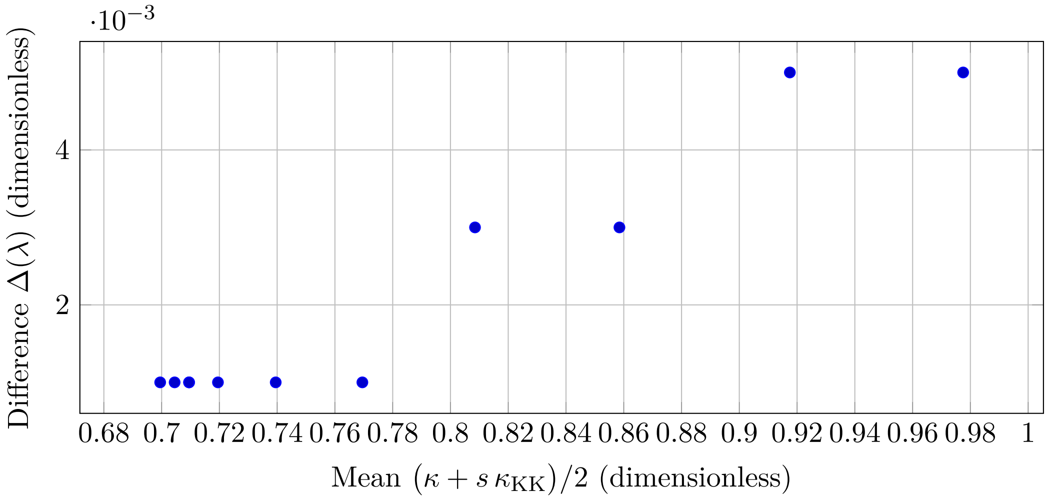

Figure 3: Bland–Altman style plot: residual vs. mean of paired values.

6 Conclusion

Within the HSF Harmonic Scale Framework and over 135–185 nm, the KK-reconstructed dispersion aligns with the absorption-derived κ after applying $s \approx 0.981$. The observed RMS $\approx 3.21 \times 10^{-3}$ and $\rho \approx 0.989$ *indicate internal consistency within the tested window*, pending validation with full, unit-annotated data. **KK consistency is a necessary but not sufficient condition:** any causal, linear dispersion model will satisfy KK; thus these checks demonstrate internal data/model coherence rather than uniqueness of interpretation.

References

- Lewis, B.R., & Carver, J.H. (1983). Ultraviolet absorption cross sections for CO_2 at 370 K, 121–190 nm.
- Yoshino, K., *et al.* (1996). Absolute absorption cross sections for CO_2 in the 120–175 nm region at 195 K.
- Standard references on Kramers–Kronig relations in dispersion theory.

DOI: 10.5281/zenodo.16921424