

Drift-Aware, Chirp-Controlled Photonic Biasing in Topochemically Constrained Polymerization of Furan Crystals: A Pre-Registered Experimental and Statistical Framework

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Abstract

The high-pressure polymerization of molecular precursors into carbon nanothread structures represents a frontier in materials synthesis, offering pathways to one-dimensional materials with exceptional mechanical and electronic properties. This manuscript presents a comprehensive, pre-registered experimental framework designed to evaluate whether chirped two-photon excitation (TPA) can influence reaction outcomes in compressed furan crystals under extreme pressure conditions (5–10 GPa).

The proposed study integrates multiple methodological innovations: controlled photonic excitation spanning ultraviolet and femtosecond laser modalities, drift-aware statistical modeling to account for systematic temporal variations, Bayesian inference with rigorous prior predictive validation, interleaved experimental sequencing to control for confounding variables, and noise-floor calibration through extended control-only runs.

Importantly, this work makes no claims regarding anticipated outcomes. Rather, it establishes the precise conditions, statistical thresholds, and decision criteria under which claims about photonic biasing of topochemical reactions can be rigorously tested. By pre-registering our analytical approach, we aim to prevent post-hoc hypothesis generation and ensure that any conclusions drawn from the eventual data rest on firm statistical foundations.

1 Introduction

The synthesis of carbon nanothreads through high-pressure polymerization of aromatic and heteroaromatic molecular precursors has emerged as a transformative approach to creating one-dimensional carbon allotropes with properties distinct from both graphene and diamond. Since the first successful synthesis of diamond nanothreads from benzene under pressure exceeding 20 GPa, the field has expanded to investigate alternative precursors that might yield threads with tunable electronic properties, enhanced stability, or more facile synthesis conditions.

Furan, a five-membered heteroaromatic compound containing oxygen, presents a particularly intriguing precursor candidate. The oxygen heteroatom introduces both electronic perturbations and structural constraints that differentiate furan from its all-carbon analogs. Under compression within a diamond anvil cell (DAC), furan molecules can potentially polymerize through [4+2] cycloaddition reactions or alternative pathways, forming extended thread-like structures with incorporated oxygen atoms. Such heteroatom-doped nanothreads might exhibit modified band gaps, altered mechanical flexibility, or enhanced chemical reactivity compared to pure carbon threads.

The polymerization of furan and related heterocycles occurs under topochemical constraints—the crystal packing geometry and available free volume fundamentally limit which reaction pathways are sterically accessible. This topochemical control is generally viewed as deterministic: given a specific crystal structure and pressure-temperature conditions, the reaction pathway is constrained to those

transformations that maintain the integrity of the crystalline lattice. However, recent experimental and theoretical work has suggested that external perturbations, including electromagnetic fields and photonic excitation, may influence reaction probabilities even within these constrained environments. The mechanism remains unclear—whether photonic excitation temporarily distorts the potential energy surface, creates transient excited states with modified reactivity, or simply provides the activation energy to overcome kinetic barriers that would otherwise be insurmountable.

This ambiguity motivates the present study. We seek to determine whether photonic excitation, specifically through two-photon absorption using chirped femtosecond pulses, can bias the outcome of high-pressure furan polymerization. If such biasing is observed, it would suggest that topochemical constraints, while restrictive, are not absolute determinants of reaction pathways. If no effect is detected despite adequate statistical power, this would support the dominance of geometric constraints in controlling solid-state reactivity.

The choice of chirped two-photon excitation is deliberate. Chirp—the temporal ordering of frequencies within an ultrafast pulse—provides a control parameter absent from continuous-wave or unchirped pulsed excitation. Negative group delay dispersion (GDD) places higher frequencies at the leading edge of the pulse, while positive GDD places them at the trailing edge. This temporal ordering can, in principle, interact with the coherent dynamics of excited states, potentially steering population through different pathways on the potential energy surface. By systematically varying chirp while holding pulse energy, duration, and center wavelength constant, we can isolate the specific contribution of pulse temporal structure to reaction outcomes.

This manuscript represents a pre-registration of our experimental and analytical protocol. We specify in advance the experimental conditions, measurement procedures, statistical models, decision criteria, and failure modes. This approach guards against the temptation to reformulate hypotheses after observing data—a practice that, while common, fundamentally undermines the epistemic value of statistical inference. By committing to our analytical framework now, we ensure that whatever conclusions emerge will be interpretable within the frequentist or Bayesian paradigms we have adopted.

2 Research Question and Hypothesis

2.1 Primary Research Question

The central question motivating this investigation is: **Does photonic excitation modality influence the probability of nanothread formation in compressed furan crystals?**

This question encompasses several subsidiary inquiries:

- Does two-photon excitation at 650 nm produce different reaction outcomes than single-photon ultraviolet excitation at 355 nm, when both are calibrated to deposit equivalent energy densities?
- Does the chirp of femtosecond pulses affect reaction yields or product distributions?
- Are observed effects, if any, attributable to specific pulse parameters rather than generic thermal or pressure perturbations?

2.2 Hypothesis

We formulate our hypothesis in probabilistic terms:

$$P(\text{Outcome}|\text{TPA}) \neq P(\text{Outcome}|\text{UV}) \tag{1}$$

where “Outcome” refers to the measured state of the furan sample following excitation, encompassing both the presence or absence of polymerization products and the structural characteristics of any threads formed. The conditioning on TPA versus UV represents the experimental manipulation of excitation modality while holding other parameters as constant as feasible.

The null hypothesis, which we will attempt to falsify, asserts that the excitation modality has no effect on reaction outcomes beyond what would be expected from the deposited energy alone:

$$H_0 : P(\text{Outcome}|\text{TPA}) = P(\text{Outcome}|\text{UV}) \quad (2)$$

3 Experimental System

3.1 Diamond Anvil Cell Configuration

All high-pressure experiments will be conducted using a symmetric diamond anvil cell with standard design features modified for optical access. The cell will be equipped with beveled diamond anvils having culet diameters of 300 μm , permitting sample compression to pressures exceeding 10 GPa while maintaining optical transparency for both excitation and probe beams.

Pressure Range. The primary experimental window spans 5–10 GPa. This range is selected based on prior literature suggesting that furan polymerization initiates in this regime while remaining below conditions where irreversible decomposition or diamond failure becomes probable. Within this window, we will conduct experiments at multiple discrete pressure points to assess pressure-dependent effects.

Pressure Calibration. Pressure will be determined in situ using the ruby fluorescence method. Small ruby chips (approximately 5 μm diameter) will be co-loaded with the furan sample, and the R1 fluorescence line will be excited with low-power 532 nm light. The pressure-dependent wavelength shift will be converted to pressure using the non-linear calibration formula appropriate for the 5–10 GPa range. Calibration measurements will be performed before and after each experimental sequence, with interpolation used to estimate pressure during runs.

Pressure Medium. An inert pressure-transmitting medium is essential to maintain hydrostatic conditions and prevent chemical contamination. We will use either argon or neon, loaded cryogenically as liquids and solidified under compression. Argon provides adequate hydrostaticity to approximately 10 GPa, while neon extends this range further. The choice between media will be based on availability and specific experimental requirements.

Drift Constraint. Pressure stability is critical for interpreting results, as pressure variations can themselves induce phase transitions or reaction progress. We impose the following drift constraint:

$$|P(t) - P_0| < 0.1 \text{ GPa} \quad (3)$$

where P_0 is the target pressure at the beginning of an experimental run. If pressure drift exceeds this threshold during a measurement sequence, the data from that sequence will be flagged for separate analysis or exclusion, depending on the magnitude and pattern of drift.

3.2 Sample Preparation

The quality of starting materials fundamentally constrains the interpretability of any high-pressure synthesis experiment.

Furan Purity. Commercial furan will be purified to $\geq 99.9\%$ purity through fractional distillation under inert atmosphere. Purity will be verified by gas chromatography-mass spectrometry (GC-MS) and proton nuclear magnetic resonance (^1H NMR) spectroscopy. Residual water and oxygen are particularly problematic, as they can initiate unwanted side reactions or degrade the sample during loading.

Crystal Size and Selection. Single crystals of furan will be grown through controlled cooling of the liquid in capillary tubes. Target crystal dimensions range from 10–50 μm in lateral extent, with thicknesses less than 20 μm . These dimensions ensure adequate optical penetration while maintaining the bulk crystalline properties essential for topochemical control. Crystals will be selected under a polarizing microscope for optical uniformity and absence of visible defects.

Pre-characterization. Each crystal will be characterized by X-ray diffraction (XRD) and Raman spectroscopy before compression to establish baseline structural and vibrational properties. The XRD pattern will confirm crystallinity and phase identity, while Raman spectroscopy provides reference spectra for subsequent pressure-induced changes. These baseline measurements are essential for distinguishing photonic effects from pressure-induced transformations.

4 Excitation System

4.1 Two-Photon Absorption Configuration

The TPA excitation system centers on a regeneratively amplified Ti:sapphire laser producing 120 fs pulses at 800 nm, with subsequent optical parametric amplification (OPA) to generate tunable visible output.

- **Wavelength:** The excitation wavelength is set to 650 nm, corresponding to the second harmonic of the OPA idler. This wavelength is chosen to provide photon energies insufficient for single-photon excitation of furan (which has its first electronic absorption band below 300 nm) while enabling two-photon absorption to populate higher-lying excited states. The 650 nm light also penetrates the diamond anvils with minimal loss.
- **Pulse Duration:** The transform-limited pulse duration is 120 fs. Chirping will extend the temporal envelope, but the Fourier-transform-limited duration establishes the bandwidth and peak intensity relationships.
- **Repetition Rate:** A repetition rate of 10 kHz balances the need for adequate signal accumulation against thermal management concerns. At this rate, successive pulses arrive at 100 μs intervals, providing sufficient time for thermal diffusion between pulses while maintaining experimental efficiency.
- **Pulse Energy:** Pulse energies will range from 0.2–3.8 μJ , corresponding to peak intensities at the focal spot of approximately 10^{11} – 10^{13} W/cm^2 . This range spans from below the threshold for observable two-photon effects to intensities where multiphoton ionization or optical damage might become concerns. The upper limit is set by the thermal constraint described in Section 5.
- **Beam Waist:** The excitation beam will be focused to a waist of 5–10 μm using a long-working-distance objective lens external to the diamond anvil cell. This spot size is comparable to the crystal thickness, ensuring relatively uniform excitation through the sample while providing spatial selectivity for Raman probing.

4.2 Ultraviolet Control Condition

The UV control experiments will use the third harmonic (355 nm) of a Nd:YAG laser or equivalent source. This wavelength corresponds to photon energies (3.49 eV) exceeding the first electronic transition of furan, enabling direct single-photon excitation. By comparing outcomes under UV versus TPA excitation at equivalent deposited energy densities, we can isolate effects specific to the excitation mechanism (simultaneous two-photon absorption versus sequential single-photon processes).

The UV beam will be spatially filtered and focused to match the TPA beam profile as closely as possible. Pulse energies will be scaled to match the two-photon excitation probability, accounting for the different absorption cross-sections.

4.3 Chirp Control Protocol

Chirp manipulation provides the primary experimental variable for investigating pulse-structure effects.

Group Delay Dispersion (GDD) Values. We will test four GDD conditions:

- **Negative GDD:** The pulse is arranged such that higher frequencies precede lower frequencies. This “up-chirp” can favor adiabatic following in certain excitation schemes.
- **Zero GDD:** The transform-limited pulse with minimal temporal duration and maximal peak intensity.
- **Positive GDD:** Lower frequencies precede higher frequencies. This “down-chirp” can create transient population inversions or modify multiphoton excitation pathways.
- **Extended Sweep:** GDD values of $\pm 2\times$ the standard range, testing whether chirp effects, if observed, show monotonic dependence on dispersion magnitude.

Chirp will be introduced using a pair of fused silica prisms or a grating-based pulse shaper, with GDD calibrated through frequency-resolved optical gating (FROG) or spectral phase interferometry for direct electric-field reconstruction (SPIDER).

5 Thermal Management and Constraints

Photonic excitation inevitably deposits energy into the sample, raising local temperatures and potentially inducing thermal reactions indistinguishable from photochemical processes. Rigorous thermal constraints are therefore essential for interpretable results.

5.1 Temperature Rise Estimation

The temperature increase per pulse can be estimated from the deposited energy and sample thermal properties:

$$\Delta T = \frac{\alpha E}{\rho C_p V} \tag{4}$$

where:

- α is the fraction of pulse energy absorbed (dependent on two-photon cross-section and concentration)

- E is the pulse energy (J)
- ρ is the furan density (kg/m^3)
- C_p is the specific heat capacity ($\text{J}/\text{kg}\cdot\text{K}$)
- V is the excitation volume (m^3)

For typical parameters ($E = 1 \mu\text{J}$, $V \approx 10^{-15} \text{ m}^3$, $\rho \approx 1000 \text{ kg}/\text{m}^3$, $C_p \approx 1500 \text{ J}/\text{kg}\cdot\text{K}$, $\alpha \approx 0.1$), the temperature rise per pulse is approximately 0.7 K.

5.2 Thermal Constraint

We impose the constraint:

$$\Delta T < 1 \text{ K per pulse} \quad (5)$$

This threshold is selected to ensure that thermal effects remain negligible compared to the photonic excitation effects we seek to investigate. At temperature rises below 1 K per pulse, thermal reaction rates (which typically follow Arrhenius behavior with activation energies of 0.5–1 eV) increase by less than 10% between pulses, insufficient to explain substantial reaction yields without invoking photonic mechanisms.

If higher pulse energies are required for observable signals, we will reduce repetition rate or implement active cooling strategies rather than violate this constraint.

6 Experimental Design

6.1 Interleaved Sampling Protocol

To control for temporal drift in experimental conditions (laser power fluctuations, pressure creep, sample degradation), we employ an interleaved sampling design:

$$\text{UV} \rightarrow \text{TPA} \rightarrow \text{Chirp+} \rightarrow \text{Chirp-} \rightarrow \text{repeat}$$

Each “block” consists of sequential measurements under these four conditions, with the order randomized across blocks to prevent systematic bias from time-dependent confounders. This interleaving ensures that slow drift affects all conditions approximately equally, allowing drift effects to be separated from condition effects in the statistical analysis.

The number of blocks will be determined by power analysis (see Section 9), but we anticipate 20–50 blocks per pressure condition, yielding 80–200 measurements per experimental parameter.

6.2 Noise Control

A critical component of any detection experiment is establishing the noise floor—the level of signal variation expected in the absence of any experimental manipulation. We will conduct extended control runs under the following conditions:

No-Excitation Control. The sample will be maintained at target pressure for 10 hours without any photonic excitation beyond the weak probe beams used for Raman and ruby fluorescence measurements. Raman spectra will be collected at intervals matching the experimental sampling rate. Any changes observed during this period represent pressure-induced evolution, thermal drift, or instrumental instability rather than photonic effects.

Probe-Only Control. The Raman probe beam (typically 532 nm at mW power levels) will be applied at the same temporal pattern as the excitation beams in the main experiment. This control tests whether the probe itself induces photochemistry.

These control runs will establish the baseline variability against which photonic effects must be distinguished.

7 Measurement Methods

Three complementary techniques will characterize the sample state:

7.1 Raman Spectroscopy

Raman spectroscopy provides vibrational fingerprints of molecular structure and bonding. We will focus on:

- The C=C stretching region ($1500\text{--}1700\text{ cm}^{-1}$) to monitor aromatic ring integrity
- The C–O–C stretching region ($1000\text{--}1100\text{ cm}^{-1}$) sensitive to furan ring opening
- Low-frequency lattice modes ($< 500\text{ cm}^{-1}$) indicating crystalline order
- New modes appearing in the $1200\text{--}1400\text{ cm}^{-1}$ range characteristic of sp^3 carbon formation in nanothreads

Spectra will be collected using a confocal Raman microscope with 532 nm excitation at power levels below 1 mW to avoid sample perturbation. Acquisition times of 30–60 seconds will provide adequate signal-to-noise while minimizing probe exposure.

7.2 X-ray Diffraction

XRD provides direct structural information about crystalline phases and their evolution. Using synchrotron radiation (or a laboratory micro-source if synchrotron access is unavailable), we will monitor:

- The positions and intensities of Bragg peaks from the furan crystal
- The emergence of new diffraction features indicating polymerization products
- Changes in lattice parameters reflecting molecular rearrangement

XRD measurements will be performed before compression, after reaching target pressure, and following photonic excitation sequences.

7.3 Ruby Fluorescence

In addition to pressure calibration, ruby fluorescence provides a local temperature probe through the temperature dependence of the R1 line width and position. This enables verification that thermal constraints are maintained and allows correction for minor temperature variations in the analysis.

8 Data Collection Protocol

All experimental parameters will be logged continuously to enable retrospective analysis and drift correction:

Time-Resolved Measurements. Raman spectra will be collected at fixed intervals (every 5 minutes during excitation sequences, every 30 minutes during control runs) to track reaction kinetics.

Continuous Logging. The following parameters will be recorded at 1 Hz or higher:

- Pressure (from ruby fluorescence)
- Sample temperature (from ruby line shape analysis)
- Laser pulse energy (via photodiode monitoring)
- Laser center wavelength and bandwidth (via spectrometer)
- Pulse chirp (via online FROG or SPIDER)
- Ambient temperature and humidity

This comprehensive logging ensures that any anomalous results can be traced to specific experimental conditions.

9 Statistical Framework

9.1 Hierarchical Model

We employ a Bayesian hierarchical model to account for the nested structure of the data (measurements nested within blocks nested within pressure conditions). The observation model is:

$$Y_{ijt} \sim \mathcal{N}(\mu_i + \Delta_t, \sigma_i^2 + \epsilon_j^2) \quad (6)$$

where:

- Y_{ijt} is the observed outcome (e.g., Raman intensity at a specific frequency) for condition i , block j , at time t
- μ_i is the true mean for condition i (the parameter of primary interest)
- Δ_t is a drift term capturing systematic temporal variation
- σ_i^2 is the within-condition variance
- ϵ_j^2 is the between-block variance

The inclusion of separate drift (Δ_t) and block (ϵ_j) terms allows us to model and remove systematic variation unrelated to the experimental manipulation.

9.2 Prior Distributions

We specify weakly informative priors based on the scale of expected effects:

$$\mu_i \sim \mathcal{N}(0, 5) \tag{7}$$

This prior centers the condition means at zero (corresponding to standardized outcome measures) with a standard deviation of 5, permitting substantial effects while providing enough regularization to prevent extreme estimates from noisy data.

$$\sigma_i \sim \text{HalfNormal}(2) \tag{8}$$

The half-normal prior on standard deviations reflects our expectation that measurement variability will be moderate, with 95% probability mass below approximately 4 units.

9.3 Decision Criterion

We will conclude that photonic excitation modality influences reaction outcomes if:

$$P(\mu_{\text{TPA}} - \mu_{\text{UV}} > \delta) > 0.95 \tag{9}$$

where δ is a pre-specified effect size representing the minimum scientifically meaningful difference. We set δ at 0.5 standardized units, corresponding to a “medium” effect in Cohen’s terminology. The 95% probability threshold corresponds to conventional frequentist significance levels while providing direct probabilistic interpretation.

9.4 Prior Predictive Checking

Before analyzing experimental data, we will simulate 1000 datasets from the prior predictive distribution under the null hypothesis (no condition effects). For each simulated dataset, we will compute our decision criterion. The proportion of simulations in which the criterion is satisfied represents the expected false positive rate under the null. If this rate deviates substantially from 5%, we will revise our priors or decision threshold.

10 Error and Drift Modeling

Systematic errors and temporal drift pose significant threats to internal validity in longitudinal experiments. Our framework addresses these through multiple mechanisms:

Drift Term (Δ_t). The drift term in our statistical model captures smooth temporal variation using a Gaussian process or spline basis. This allows us to model slow changes in experimental conditions (laser power drift, pressure creep) without assuming specific functional forms.

Measurement Noise (ϵ_j). Block-level random effects account for variation between experimental blocks that may arise from subtle differences in sample positioning, pressure gradients, or laser alignment.

Systematic Error Tracking. We will maintain a detailed error log documenting any deviations from protocol, equipment malfunctions, or environmental perturbations. These will be coded as covariates in exploratory analyses.

11 Reproducibility Protocol

Scientific claims are only as credible as the evidence supporting them, and reproducibility is the cornerstone of credible evidence. We commit to:

Full Parameter Disclosure. All experimental parameters not explicitly varied as independent variables will be reported, including laser manufacturer and model, optical component specifications, purification protocols, and environmental conditions.

Open Statistical Model. The complete Stan or PyMC code for our Bayesian analysis, including prior specifications, will be made available through a public repository prior to data collection.

Repeatability. The entire experimental sequence will be performed in duplicate on separate days with independently prepared samples. Results will be considered reliable only if both replicates yield consistent conclusions.

Independent Validation. We encourage independent laboratories to attempt replication using the protocols specified herein. Any deviations from our protocol in replication attempts will be documented and analyzed as potential moderators of effect size.

12 Risk Analysis

Multiple factors could compromise the validity of our conclusions:

Thermal Artifacts. If our thermal constraints are violated, observed effects may reflect thermal chemistry rather than photonic biasing. We mitigate this through continuous temperature monitoring and strict pulse energy limits.

Pressure Drift. Pressure variations during experiments could induce phase transitions or reaction progress independent of photonic excitation. The interleaved design and drift modeling provide protection, but substantial drift may necessitate exclusion of affected data.

Optical Damage. High-intensity femtosecond pulses can damage diamond anvils or create permanent color centers that interfere with spectroscopic measurements. We will inspect anvils before and after each run and exclude data if damage is detected.

Signal Degradation. Extended laser exposure may photobleach the sample or induce cumulative damage that obscures the signals of interest. The interleaved design distributes such degradation across conditions, but severe degradation may limit experimental duration.

13 Failure Modes

We explicitly acknowledge several ways in which this study might fail to achieve its objectives:

Null Result. We may find no evidence that photonic excitation modality influences reaction outcomes. This would be a scientifically valuable result, supporting the dominance of topochemical constraints, provided our statistical power was adequate to detect plausible effect sizes.

Drift-Dominated Outcome. If temporal drift or measurement noise exceeds anticipated levels, we may be unable to distinguish condition effects from background variation. This would indicate a need for improved experimental stability or larger sample sizes.

Insufficient Signal. The Raman or XRD signals associated with nanothread formation may be too weak to quantify reliably under our experimental conditions. This would necessitate alternative detection strategies or longer integration times.

Chirp Irrelevance. Even if TPA influences reaction outcomes, the specific chirp of the pulses may have no detectable effect. This would suggest that the excitation mechanism involves incoherent processes insensitive to pulse temporal structure.

14 Conclusion

This manuscript presents a comprehensive, pre-registered framework for investigating whether photonic excitation can bias reaction outcomes in topochemically constrained systems. By specifying our experimental parameters, statistical models, and decision criteria in advance, we ensure that whatever conclusions emerge from this study will rest on firm methodological foundations.

We make no predictions about the outcome. The value of this work lies not in confirming or refuting a specific hypothesis, but in establishing the conditions under which such hypotheses can be rigorously tested. Whether photonic biasing of topochemical reactions proves to be a real phenomenon or a methodological artifact, the field will advance through carefully designed experiments like the one described herein.

The pre-registration format may be unconventional, but it reflects our commitment to scientific integrity. In an era of reproducibility crises and questioned research practices, transparency about methods, analysis plans, and potential failure modes is not merely commendable—it is essential. We invite scrutiny of this protocol and welcome suggestions for improvement before data collection commences.

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