Cubic Organic Scintillators as Improved Materials for Fast Neutron Detection (FY12-FY13)

Sandia National Laboratories
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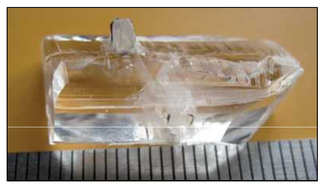
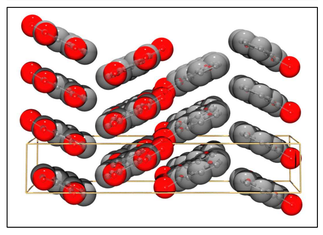
Problem

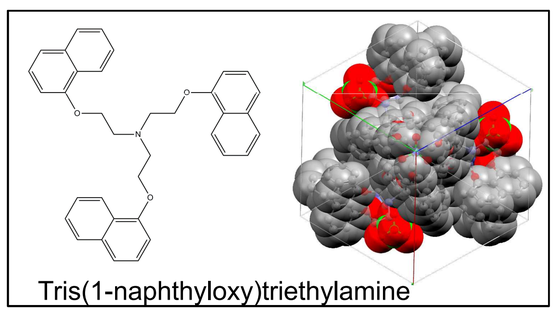




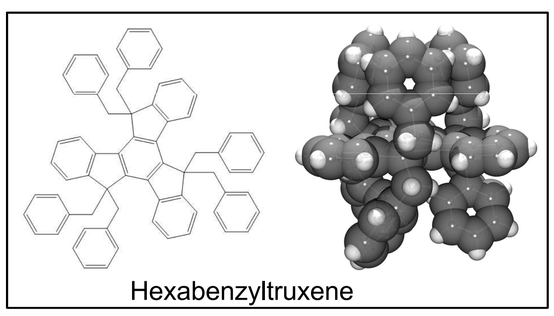
- Existing organic scintillator crystals possess several limitations:
  - Mechanical instability/fragility
  - Anisotropic light output
  - Limited particle discrimination capabilities
  - Slow and/or difficult crystalline growth
  - Afterglow effects that limit count-rate
- All known examples crystallize in low-symmetry monoclinic space groups
  - Limited synthetic flexibility and structure-property understanding
- Outlook for improved materials is extremely limited
  - Same compounds have been used since 1950's
  - Lack of fundamental understanding: present approaches are empirical vs. hypothesis based

Approach

- Synthesize C_3-symmetric compounds to increase molecular and crystallographic symmetry
  - Survey of CSD indicates less than 0.1% of organic crystals are cubic
  - Large proportion of cubic examples possess three-fold molecular site symmetry
  - Synthesize compounds based upon various core structures
    - Enables crystal engineering of new compounds that are composed of efficient chromophores
- Symmetry effects are well known but have not been applied to scintillators
  - Second-rank tensor properties
  - Examples:
    - Particle Discrimination: Largely 2-D exciton transport in monoclinic structures, versus 3-D transport in higher symmetry materials
    - Crystal Growth and Ruggedization: Robust 'metal-like' mechanical properties for cubic organic crystals
    - Neutron spectrometery: Isotropic light output



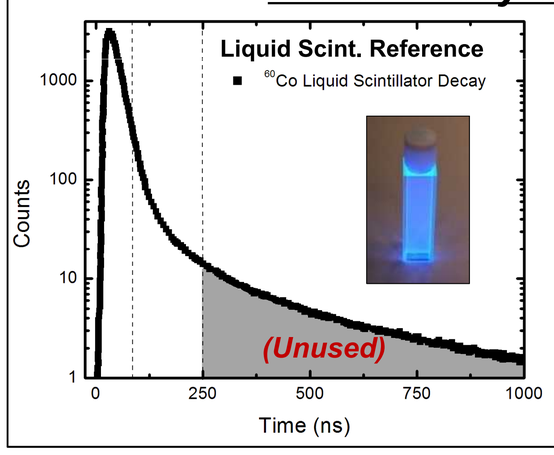
Tris(1-naphthyloxy)triethylamine

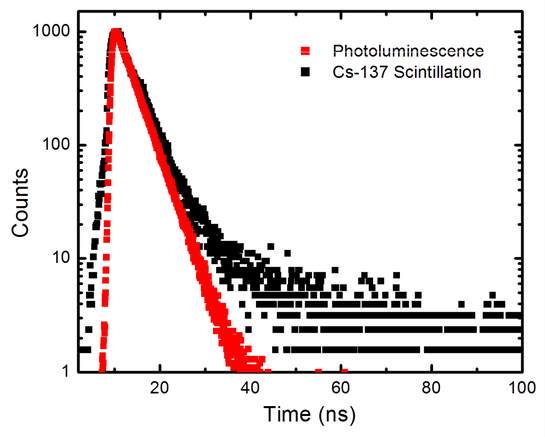


Hexabenzyltruxene

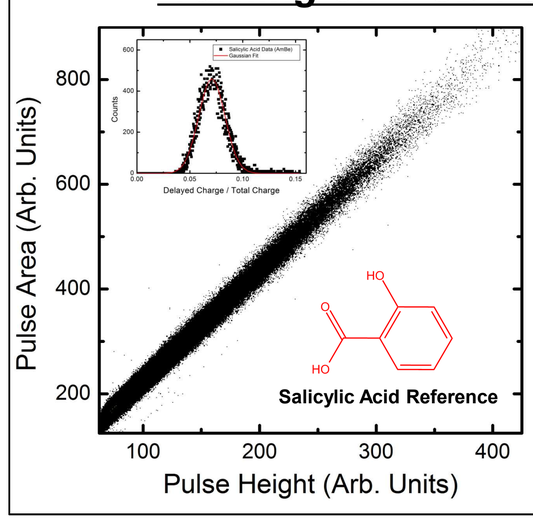
Results

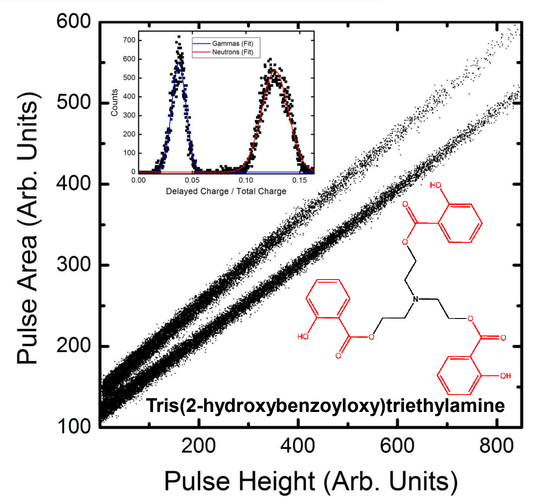
Faster Decay Characteristics

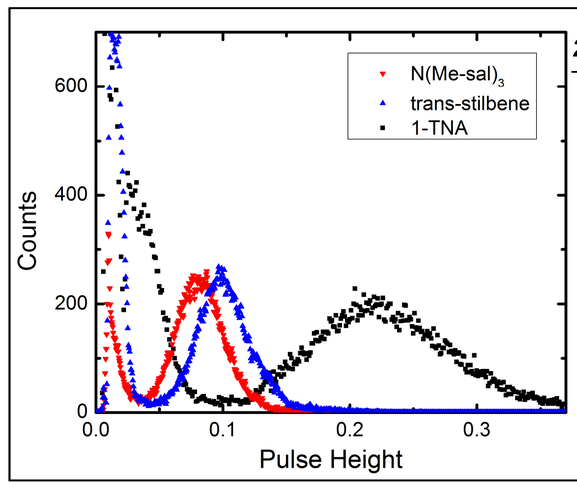




'Turning on' PSD Particle Discrimination







^{241}Am Light-Yield Comparison

- Comparable light yields and alpha energy resolution relative to *trans*-stilbene benchmark
- Broad PHS for 1-TNA possibly due to oxidized impurities and/or self-absorption

Significance

- Generalized design approach enables targeted synthesis of improved fast-neutron scintillators
- Initial findings indicate dramatically improved particle-discrimination performance
- Findings provide the first rational approach to new organic scintillator crystals
  - 'Re-purposing' efficient chromophores that were previously discounted due to low PSD and/or difficult crystal growth
    - p-terphenyl and PPO, respectively

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