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Technical Notes

Scintillator Library: A database of inorganic and organic scintillator properties

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ABSTRACT

The Scintillator Library (scintillator.lbl.gov) is a database of scintillator properties hosted by Lawrence Berkeley National Laboratory in a web-accessible format. It contains a variety of measured inorganic and organic scintillator properties extracted from peer-reviewed literature and manufacturer specifications. Data housed within the Scintillator Library supply an important resource for developers of scintillator-based detection systems and an aid for scientists seeking to establish connections between fundamental material and chemical properties and the associated scintillation performance.

Scintillators play an important role in basic science investigations and support a variety of applications, from medical imaging [1] to geophysical surveys [2] to countering nuclear threats [3]. Despite their widespread use, a complete first-principles description of the molecular characteristics and physical processes that give rise to various scintillator properties is lacking [4,5]. As a result, the development of new scintillators has largely proceeded via serendipity or a “cook and look” approach [4]. The development of scintillator-based detection systems is also hampered by the lack of accessible data on performance parameters needed to inform design decisions. This hinders the ability to fully consider material properties in the optimization of detection systems and often leads to material characterization being conducted as part of the detector development process. To provide a basis for addressing these challenges, the Scintillator Library [6] is a web-based resource supplying a compilation of inorganic and organic scintillator material properties. This database, hosted by Lawrence Berkeley National Laboratory (LBNL), provides direct access to data extracted from manufacturer specification sheets and peer-reviewed literature, along with citations and links to the original manuscripts.

The Scintillator Library was originally created for inorganic media with support from a Department of Homeland Security (DHS) project focused on high-throughput synthesis and characterization of inorganic scintillators [7]. Over the course of this work, a facility was founded at LBNL with the aim of accelerating the discovery and development of new inorganic scintillating materials that offer outstanding energy resolution and can be produced cost-effectively at scale. All synthesis and measurement data from this facility were stored in an internal database, which then graduated to a public database featuring the most promising compounds examined in the study as well as inorganic scintillator data extracted from the available literature.

In its current incarnation, the Scintillator Library is comprised of two primary databases — the Inorganic Library and Organic Library — as depicted in Fig. 1. The Inorganic Scintillator Library provides detailed specifications on a wide range of inorganic scintillators, including both crystals and crystalline powders as well as ceramics, with more than 600 entries currently available. Properties tabulated include the material density, luminosity, emission time, peak emission wavelength, and other characteristics detailed in Fig. 1. Where data are available, emissions from different mechanisms are tabulated separately (e.g., characteristics of BaF_2 emission via self-trapped excitons, core-valence transitions, and a Ce^{3+} luminescent activator ion [8,9] each have independent entries). Data in the Inorganic Scintillator Library have been used to support a range of studies, including the review of detection media for positron emission tomography instrumentation [10], the evaluation of radioisotope identification devices for homeland security threat assessment [11], and the pursuit of high-quality images from proton radiography experiments [12].

The Organic Scintillator Library, introduced in 2023, provides manufacturer specifications and quenching data for a wide variety of organic crystals, liquids, plastics, and glasses. Properties tabulated are detailed in Fig. 1. Of particular interest for neutron detection applications are the ionization quenching data, which include a compilation of organic scintillator response to electrons, protons, and heavier ions as a function of energy. For some organic scintillators, quenching data pages are provided with plots of the measured light yield data,

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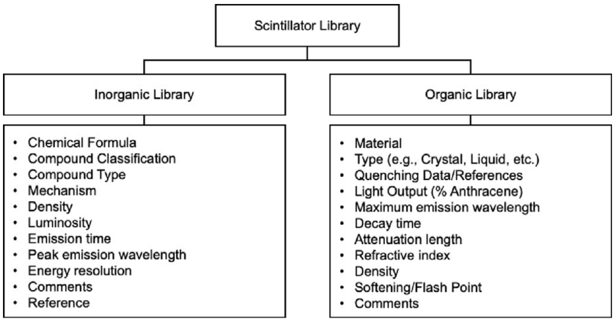

Fig. 1. Schematic diagram illustrating library structure and core components.

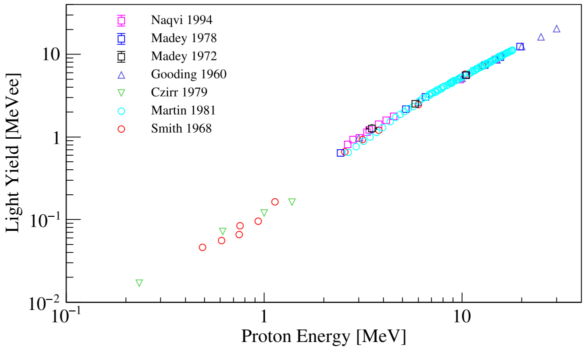

Fig. 2. Measured EJ-212 light yield data in MeVee as a function of proton energy [25–31].

showcasing particle light yield relations from all referenced papers in a single graphic. For example, Fig. 2 shows the compiled proton light yield data for EJ-212, a plastic organic scintillator from Eljen Technology [13] and commercial equivalent of the Luxium BC-400 [14] and the former Nuclear Enterprises NE 102A.[1] Text files are included that report the extracted data along with details on the experimental setup such as photodetector type and model, signal acquisition and processing, light output calibration procedures, and light yield extraction methods.

The quenching data pages within the Organic Scintillator Library enable direct comparison of the available literature measurements, both visually and quantitatively, which allows for assessment of the current state of understanding of the ionization quenching behavior of a particular material. Discrepancies observed between the different reported light yield measurements may be explained in part by differences in the integration lengths used to measure the light output [16], methodological errors in digital signal processing [17], unaccounted for nonlinearity in the photodetector response [18], bias associated with characterization of the Compton edge used for light output calibration [19], and bias associated with the edge characterization method used by some authors [20]. Often overlooked, nonproportionality of the electron light yield may also introduce further biases in light output calibration or conversion to the MeVee light unit [21–23]. In this regard, the Organic Scintillator Library provides an important resource for experimental details, analytical methods, and measurement uncertainties and may facilitate generation of a measurement template with reporting standards (akin to those developed for more traditional nuclear data measurements [24]).

The Scintillator Library provides value to the nuclear science and radiation detection communities in a variety of capacities. Primarily, the library can be used to guide scintillating media selection for specific applications, both in terms of general screening of material properties as well as via input of library data to Monte Carlo simulations predicting scintillator-based detector performance. For example, the unified model in Geant4 [32] allows for optical photon simulation, taking as input parameters such as the scintillation yield, refractive index, and attenuation length of the scintillating medium [33]. In the case of organic scintillators, the response to neutron and charged particle interactions in scintillator-based detectors can be simulated using particle transport codes and the tabulated quenching data [34]. The library further provides a guidepost for future material characterization efforts by highlighting gaps in the available literature.

The Scintillator Library also lays the foundation for data evaluation and theory development. Data evaluation is the process by which experimental measurements and theoretical calculations are jointly considered to provide a recommended data value. In the case of nuclear reaction cross section evaluation, for example, the Experimental Nuclear Reaction Data (EXFOR) library serves as the primary repository for measured nuclear reaction cross section data and thereby plays a key role in supporting the evaluation process [35]. In a similar capacity, the Scintillator Library provides a stepping stone towards recommended values of important scintillator properties. The data compiled within the Scintillator Library may also be used to support the development of theoretical models connecting chemical and material properties to scintillation performance, by acting as a benchmark for model evaluation or by informing the development of semi-empirical relations. For example, a comparison between (1) known cerium- and europium-activated inorganic scintillators in the Library and (2) activator $4f$ and $5d$ energy levels estimated by theoretical calculations [36, 37] and empirical modeling [38] corroborate the rule that if the $4f$ level is in the valence band or the $5d$ level is in the conduction band, the activation will not be successful. Modern approaches to material discovery leverage databases of material properties for training machine learning models to predict new material stability as well as properties that might be difficult to obtain experimentally or expensive to compute [39–41]. The Scintillator Library provides a similar such resource for data-driven approaches to the extraction of scintillator properties, though future work to provide continual updates of the Scintillator Library, both in terms of database completeness and in expansion of the catalogued materials and properties, will be critical to amassing a dataset of sufficient integrity and breadth to allow for generalizable machine learning model development.

CRediT authorship contribution statement

L. Shook: Writing – review & editing, Writing – original draft, Visualization, Software, Resources, Investigation, Data curation. **T.A. Laplace:** Writing – review & editing, Writing – original draft, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **M.S. Boswell:** Writing – review & editing, Visualization, Software, Resources, Formal analysis, Data curation. **E.D. Bourret:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **S.E. Derenzo:** Writing – review & editing, Resources, Investigation, Formal analysis, Data curation. **B.L. Goldblum:** Writing – review & editing, Writing – original draft, Validation, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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[1] Proton light yield data for both NE 102 and NE 102A were included in this entry, as these materials were assumed to be sufficiently similar such that differences in ionization quenching are negligible [15].

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Data availability

Data are available online and linked in the article.

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