

## Product Information

### Poly(3-hexylthiophene-2,5-diyl)

Catalog Number **698997**  
Store at Room Temperature  
Technical Bulletin AL-250

## TECHNICAL BULLETIN

CAS RN 104934-50-1  
Synonyms: P3HT; Plexcore® OS 2100

### Product Description

Plexcore OS 2100, a p-type polymer semiconductor, is a high molecular weight, highly regioregular grade of P3HT that is optimized for Organic Photovoltaics (OPV) applications. It can be combined with (6,6)-phenyl C61 butyric acid methyl ester (C60-PCBM, Catalog Number 684449, 684430, or 684457), an n-type acceptor, for use as the photoactive component of an OPV device. Performance (cell efficiencies) up to 4% [NREL (National Renewable Energy Laboratory) Certified] can be achieved with this combination. Typical p:n material ratios for OS 2100:PCBM in OPV devices range from 2:1 to 0.5:1 (w/w). A hole transport layer (HTL) is required for efficient hole carrier extraction when using OS 2100 in an OPV device. Therefore, the use of an HTL for use in OPV device development is strongly recommended.

Other acceptors are available commercially and many fullerene derivatives, as well as others molecules, have been reported in the open literature. For other n-type acceptors the p:n ratios must be optimized for the device performance.

OPV lifetime measurement is an emerging science and standardized test methods are not available. The standardization of OPV lifetime is being evaluated. Well encapsulated devices, stored under ambient conditions, are stable for many months, with the ultimate lifetime still largely unknown.

Plexcore OS 2100 has metal impurities less than 25 ppm. The specific impact of metallic impurities is dependent on which metals are present and at what concentration. There isn't a significant impact on OPV performance due to metal impurities at this stated level, although this does not rule this possibility out due to end-use application.

Purity: 99.9975% (trace metals basis)

Head-to-tail regioregularity: >98% (<sup>1</sup>H-NMR)

Fluorescence properties:  $\lambda_{\text{ex}}$  450 nm;  $\lambda_{\text{em}}$  560 nm

Molecular weight has a modest impact on OPV efficiency with the highest performance being derived from high molecular weight materials. The exact cause of this effect is not well understood.

Average  $M_n$ : 45,000–65,000

$M_w/M_n < 2$

### Precautions and Disclaimer

This product is for R&D use only, not for drug, household, or other uses. Please consult the Material Safety Data Sheet for information regarding hazards and safe handling practices.

### Preparation Instructions

Typically aromatic and halogenated aromatic solvents are used. The product is soluble in trichlorobenzene, chlorobenzene, toluene, and xylenes. In addition, chloroform and, to a lesser degree, tetrahydrofuran (THF), are both options.

### Storage/Stability

Store the product at room temperature.

In general, conjugated organic semiconductors (like Plexcore OS) may be sensitive to some (higher energy) wavelengths of light in the presence of oxygen. While this is not an acute problem for the bulk material, solutions and thin films tend to show some sensitivity over time. Therefore, storage and handling in an inert atmosphere (like nitrogen or argon) is recommended. A yellow filter light is a standard feature for processing these materials outside of a glove box. A combination of inert atmosphere and yellow light filter is best.

## Procedure

**Note:** A yellow filter light is a standard feature for processing these materials outside of a glove box. Storage and handling in an inert atmosphere (like nitrogen or argon) is recommended.

OPV Architecture (see Figure 1):

- Transparent Substrate
- Transparent Anode – Indium/Tin Oxide (ITO)
- Hole Transport Layer (HTL)
- Photoactive Layer - P3HT:PCBM
- Cathode - Calcium/Aluminum (Ca/Al)

Preparation of P3HT:PCBM Solution (Photoactive layer):

1–2 wt% solids in various solvents or solvent blends (*o*-dichlorobenzene, chlorobenzene, toluene, *o*-xylene) with p:n (P3HT:PCBM) ratio of 2:1 to 0.5:1 (w/w).

1. Premix OS 2100 and n-type material (i.e., PCBM).
2. Dissolve mixture with suitable solvent.
3. Stir/agitate solution at 60–70 °C until well dissolved.
4. Filter solution with 0.2 µm or 0.45 µm PTFE syringe filter.

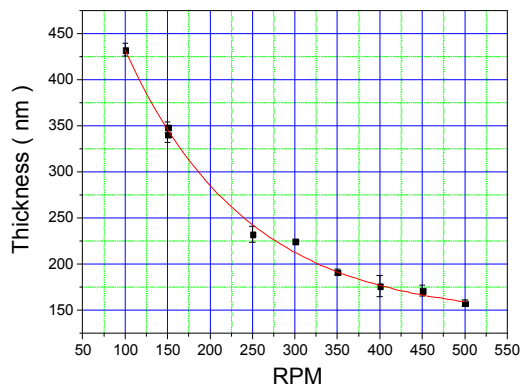
Substrate Preparation:

Prior to spin coating, typical substrate preparation might include UV/ozone treatment, air hose to remove particulates, or other surface treatments.

Photoactive Solution Deposition via Spin Coating: Spin coat photoactive solution on appropriate substrate. Each spin coater is different; see Figure 2 for a general guideline of film thickness vs spin rpm.

**Figure 2.**

Typical Spin Curve for OS2100:PCBM solution at ~2 wt % solids.



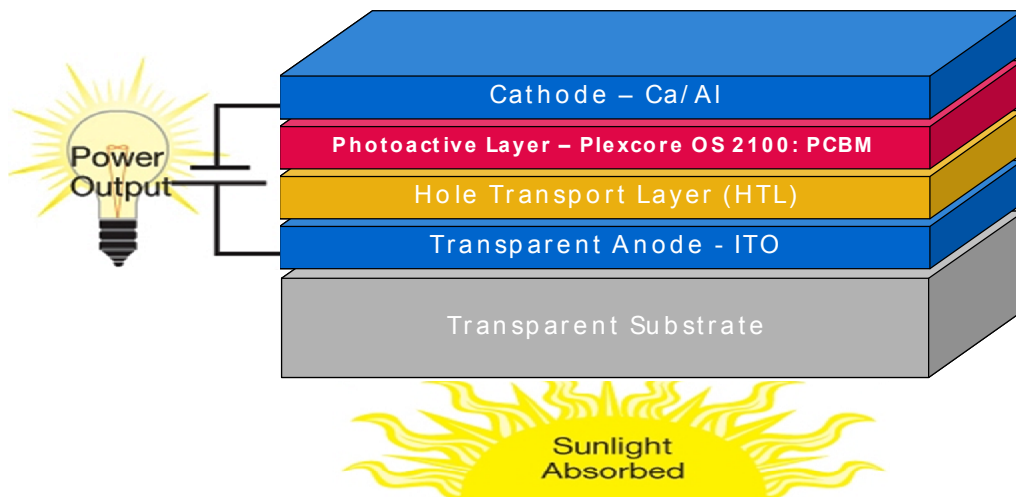
Anneal spin-coated films at 110–180 °C for up to 30 minutes in nitrogen dry box.

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**Figure 1.**

Schematic of OPV using OS 2100 - ITO: Indium Tin Oxide; Ca/Al: evaporated Calcium/Aluminum cathode



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