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Elemental analysis of novel organic semiconductor materials for molecular electronics

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1. Introduction

Organic electronics is an emerging field of technology that utilizes low cost and environmentally friendly organic materials and fabrication processes for electronic devices. Organic π-conjugated small-molecule semiconductors (pentacene, rubrene, tetracene, etc.) have become standard research materials for Organic Field Effect Transistors (OFETs).

The mechanism and characteristics of charge transport in OFETs are known to depend on the purity of the active semiconductor material and density of defects at the surfaces and interfaces [1]. Thus, development of highly pure, crystalline materials is necessary to improve the device performance and to ensure that the OFET's characteristics are not dominated by impurities, i.e. the device parameters are limited only by the intrinsic characteristics of a semiconductor.

We present a first successful attempt of application of Inductively Coupled Plasma - Mass Spectrometry (ICP-MS) to elemental analysis of organic semiconducting materials such as Rubrene, Pentacene, Tetracene, Anthracene, and Functionalized Pentacene.

2. Experimental

ICP-MS is a well-established analytical technique in the semiconductor technology for the essential trace metal characterization in chemical reagents and silicon wafers [2-3]. The ICP source, where samples are atomized and ionized, generates a strong ion current, which is instrumental in achieving exceptional detection limits. The ICP-MS instrument used in the study is PE SCIEX ELAN 6100 DRC described elsewhere [4].

All stock solutions were left for 24 hours for a better dissolving. The acids mixture HNO3/HCl (4:1 v/v) was utilized in some cases to promote the process of dissolving.

The first group of samples selected for the study consists of Sigma Aldrich as-purchased Pentacene, Rubrene, Tetracene, Anthracene (Pent-SA, Rub-SA, Tetr-SA, Anthr-SA), another group was obtained from the first group after multiple zone-refinement purification cycles in the quartz tube in presence of hydrogen gas (Rub-l, Tetr-l, Anthr-l, Anthr-ll, Anthr-lll). The samples of the second group were obtained from Rutgers University, Organic Field Effect Transistors Laboratory. The third group of samples was represented by a Functionalized Pentacene (6,13-Bis-[(triisopropylsilanyl)-ethynyl]-pentacene or TIPS) that was synthesized separately at the University of Kentucky, Synthetic Organic and Materials Chemistry Laboratory [5].

3. Discussion

The preliminary ICP-MS Standart Mode results are summarized in Table I, where the detection limits are given in (ppm) for the organic semiconductors under investigation.

It was observed that Sigma Aldrich pentacene is considerably more pure (orders of magnitude) than Rubrene original Sigma Aldrich compounds. However, it is known that pentacene performs poorly in comparison with rubrene in OFETs. This might indicate that main problem with OFET's performance actually comes from molecular impurities and structural defects, rather than from elements. Also, it is possible that because of the absence of Na which is known to be a fast diffuser in inorganic semiconductor, the performance of Rub-SA sample is improved.

4. Conclusions

All organic semiconductor molecules under investigation revealed non negligible amount of the metal contamination. Some of these metals possibly can come from the environment (dust, air pollutions) and human interference (hair, fingerprints). Clean room conditions would be

recommended for storage and any research with organic semiconductors.

The sample group after multiple zone-refinement purification cycles demonstrated a significant reduction of the metal contamination in comparison with the Sigma Aldrich as-purchased materials.

The data indicate that Pent-SA is considerably more pure (orders of magnitude) than Rub-SA compound. This is kind of unexpected, because pentacene performs much worse than rubrene in OFETs. This might indicate that main problem with OFET's performance actually comes from molecular impurities and structural defects, rather than from elements.

Also, it might indicate that because of the presence of Na in Pent-SA (which is known to be a fast diffuser in inorganic semiconductor) the performance of Rub-SA sample is better.

The elimination of the interferences is required to obtain the detection limits of some metal impurities (Fe, Cr, Zn ext.). The Dynamic Reaction Cell (DRC) Mode should be applied in future work for these purposes.

The results on elemental impurities in organic semiconductors are important for further improvement of organic semiconductor devices and experimental reproducibility. This problem deserves systematic investigation.

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Table1

Element	Pent-SA, ppm	Rub-SA, ppm	Tetr-SA, ppm	Anthr-SA, ppm	TIPS, ppm	Rub-I, ppm	Tetr-I, ppm	Anthr-I, ppm	Anthr-II, ppm	Anthr-III, ppm
Na	**25**	**-**	**-**	**9**	**105**	**-**	**-**	**8**	**-**	**6**
Mg	**2**	**191**	**-**	**1**	**8**	**-**	**-**	**-**	**-**	**-**
Al	**25**	**155**	**2**	**P**	**8**	**150**	**-**	**1**	**1**	**-**
Ti	**P**	**P**	**-**	**-**	**P**	**P**	**-**	**-**	**-**	**-**
V	**-**	**-**	**-**	**268**	**2**	**-**	**-**	**152**	**P**	**P**
Cr	**P**	**-**	**31**	**P**	**P**	**-**	**10**	**33**	**6**	**3**
Mn	**1**	**28**	**-**	**3**	**1**	**22**	**2**	**2**	**-**	**-**
Fe	**P**	**P**	**P**	**P**	**P**	**P**	**P**	**P**	**P**	**P**
Ni	**-**	**P**	**-**	**1**	**P**	**P**	**-**	**-**	**-**	**-**
Cu	**P**	**-**	**-**	**-**	**P**	**-**	**-**	**-**	**-**	**-**
Zn	**2**	**307**	**4**	**P**	**13**	**103**	**2**	**5**	**P**	**6**
Ga	**-**	**-**	**2**	**8**	**-**	**P**	**-**	**P**	**4**	**-**
Sr	**-**	**33**	**-**	**-**	**2**	**-**	**-**	**-**	**-**	**-**
Ag	**-**	**-**	**-**	**-**	**P**	**-**	**-**	**-**	**-**	**-**
Pb	**1**	**-**	**-**	**-**	**P**	**-**	**-**	**-**	**-**	**-**