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Mass Spectrometric Analyses of Two Isomeric Forms of Functionalized Pentacene Molecules SVITLANA SHCHERBYNA, DIETHARD BOHME, Dept of Physics, CMSR, York Univ., Toronto, CAN, VLADIMIR BARANOV, MDS Sciex, Concord, CAN, JOHN ANTHONY, Dept of Chemistry, Univ.of Kentucky, Lexington, USA, YORK U./SCIEX/U OF KENTUCKY TEAM — Functionalized Pentacene (FP) derivatives are one of the most interesting semiconducting organic materials for use in molecular electronics. We report a comprehensive Mass Spectrometic (MS) study of two isomeric forms of FP molecules that have recently gained considerable attention due to their high charge carrier mobility in organic thin film transistors (OTFT). Both compounds were investigated in an Electrospray Ion Source Triple Quadruple Mass Spectrometer (ESI-MS) fitted with an Ion-Molecule Reactor instead of a Collision Cell. Attempts were made to distinguish the symmetric and asymmetric isomers of FP employing differences in the rates of ion-molecule reactions, ion mobilities and Collisional Induced Dissociation (CID) patterns. In addition, the Matrix-Assisted Laser Desorption/Ionization technique (MALDI-MS) and Ion Mobility Spectrometry (IMS) were employed to study different ionization and ion transport methods prior to mass separation. IMS was able to separate the isomers only marginally. Strong ion-molecule association was observed during MALDI ionization, particularly for the symmetric FP isomer, under the reduced pressure of the source. The results of these measurements and their interpretation will be presented.

Svitlana Shcherbyna
Dept of Physics, CMSR, York Univ., Toronto, CAN

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