Travelling Wave Ion-Mobility Time-of-Flight Mass Spectrometry

Matrix assisted laser desorption ionization (MALDI) or electrospray ionization (ESI) allows the soft ionization and transfer of analytes to the gas phase. Time-of-flight (TOF) mass spectrometric analysis provides high- resolution, exact mass measurement and accurate isotope distributions of positive or negative ions for identification. This allows for chemical identification of intact molecular and cluster species, transferred from solution (ESI) or a solid matrix (MALDI).

Recent advances in technology have led to the efficient coupling of ion-mobility analysis with high resolution mass spectrometers. Ion mobility spectrometry (IMS) provides a means to separate ions based on their shape and size, providing complementary information to that obtained via standard mass spectrometry. The Synapt-G2 HDMS is the first commercial instrument of its kind, offering flexibility in terms of ion source (MALDI, nanoESI, ESI) and sample analysis, coupling a high resolution TOF mass analyzer with a travelling wave ion mobility (TWIMS) separation cell. Thus, the instrument has both the capability to obtain high resolution ESI-/MALDI-TOF mass spectra, or, with application of IMS, to obtain 2D structure-mass correlation maps. Ions of interest may also be mass selected in a quadrupole mass filter and have their individual chemistry (e.g. via collision induced dissociation) probed.

Contact

See KNMF website or contact the KNMF User Office.

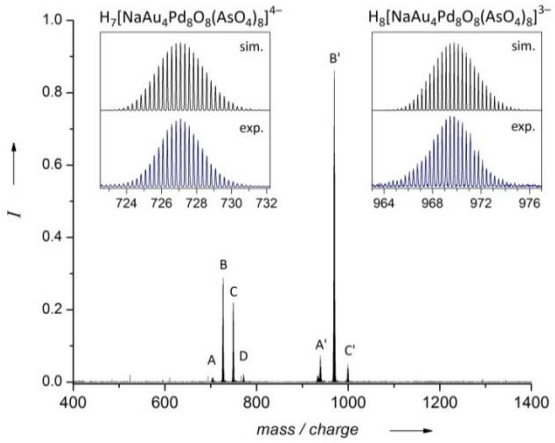
Features

- ESI/nanoESI/1kHz MALDI ion sources
- High resolution mass spectra
- 32kDa expanded mass range
- Analysis of positive and negative ions, ion chemistry
- TWIMS separation cell

Limitations/constraints

- Lower mass detection limit of: 100
- Spatial resolution of MALDI: currently 100 µm
- nanoESI/ESI: samples must be soluble.
- Air sensitive samples- the ion source is open to atmospheric conditions

Typical results



Negative-ion electrospray mass spectrum obtained from a solution of Na-Au_4Pd_8 in H_2O/DMSO. The two insets highlight peaks B and B' and compare their isotope distribution to the simulated ones for the molecular ions as labelled.

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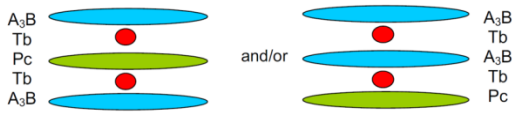
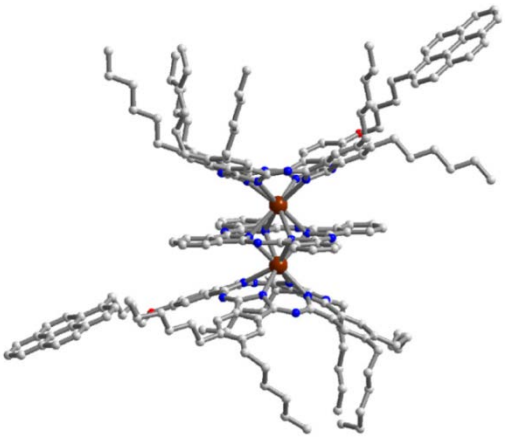
Typical results (continued)

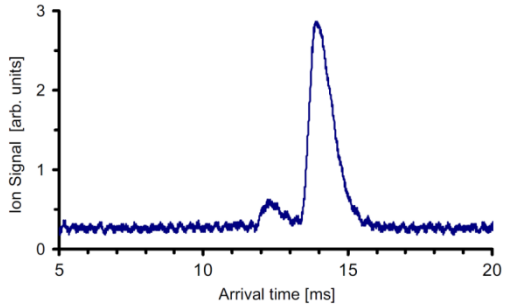
(a)



(b)



(c)



(a) Schematic structures of the two possible stacking configurations for $Tb_2(A_3B)_2Pc$ complex: a symmetric one (on the left) and an asymmetric one (on the right).
(b) Calculated structure of $(A_3B)_2PcTb_2$ (symmetric stacking)
(c) IMS arrival time distribution of the anion of $Tb_2(A_3B)_2Pc$ indicating the presence of two different isomers.

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