

Use of ion mobility mass spectrometry to study the small cobalt complexes

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Ion-mobility mass spectrometry (IM-MS) has stimulated the great research interest in structural studies of the conformations adopted by molecules. Different conformers observed in the investigated systems have been characterized by collision cross section (CCS) values evaluated from drift times in ion mobility spectra. CCS represents the effective area for the interaction between an individual ion and the contributing gas as well as delivers information about the ionic shape of the molecule. Numerous biomolecules, proteins or nucleic acids, have been already separated and characterized in the gas phase based on their mobility in a carrier buffer gas.¹⁻³ Moreover, ion mobility method has also been conducted to study smaller systems, ex. organometallic compounds with different central ions: cobalt or copper.^{4,5} The collision cross sections for these small organic compounds were calculated based on the proteins as calibrants and interesting differences in CCS values were observed depending on their shape and ligands contribution in complex formation.

Here we propose the use of IMS to evaluate the drift times of different ions brought by specified ligands around cobalt atom in hexaamine cobalt (III) chloride complex. Ion mobility spectra of cobalt complexes obtained with Synapt G2 HDMS (Waters, Manchester, UK), were recorded as a function of the cone voltage (5 V and 70 V) and the nature of the solution pH (pH 1.5, 7 and 9). Ion mobility data analysis showed that the drift time of each ion depends on the size and number of the ligands (water, amine or chlorine) coordinated with cobalt atom as well as on the experimental conditions, suggesting a structural collapse or extend. Different values of sampling cone also have impact on the shape and peaks separation. Experiments involving extended organometallic compounds, with attention to MS-MS technique, will be performed in our laboratory in the near future.

References:

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