Tandem Differential Mobility Analysis-Mass Spectrometry of the GroEL Complex: Structure Compaction in the Gas Phase and Inelastic Air-Protein Interaction

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ABSTRACT

A parallel-plate differential mobility analyzer coupled to a time-of-flight mass spectrometer (DMA-MS) is used to measure true mobility in dry atmospheric pressure air for mass-resolved electrosprayed GroEL tetradecamers (~800 kDa). Narrow mobility peaks are found (2.6-2.9% FWHM), hence, precise mobilities can be obtained for tetradecamer ions just following generation by nano-electrospray ionization. In contrast to previous studies, two conformers are found with mobilities (Z) differing by ~ 4.5% for the largest GroEL charge states (z~ 80), but by extrapolating to small z the common mobility/charge ratio Z_0/z = 0.0117 $cm^2\ V^{-1}\ sec^{-1}$ is determined for both ion populations. When interpreted as if gas-protein collisions were perfectly elastic (momentum accommodation coefficient α=0), this mobility yields a collision cross section in reasonable agreement with earlier measurements, as well as with the value expected from the native structure. However, if inelastic collisions are accounted for via the Stokes-Millikan equation using accepted values for the appropriate correction factors (α=0.91) the resulting collision cross-section decreases by ~ 36% relative to the native structure. We are able to estimate the amount of compaction for this gas-phase protein complex, for the first time, due to the symmetry of the X-ray diffraction structure, the high-resolution of the mobility measurement, and the lack of ion activation prior to mobility measurement.

KEYWORDS: Ion Mobility, Differential Mobility Analysis, GroEL, Electrospray Ionization, Protein Complexes, Mass Spectrometry