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Gas-phase complexation of α-/β-cyclodextrin with amino acids studied by ion mobility-mass spectrometry and molecular dynamics simulations

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ABSTRACT

Cyclodextrins (CDs) are a class of macrocyclic molecules that have exhibited many promising applications in various fields. The knowledge of the complexation modes and recognition mechanisms of CDs with their guests are of paramount importance for rational design of more variants with controlled properties. Herein we investigated the binding conformations and the structural characteristics of α-/β-CD with three amino acids (AA, AA=Gly, L-Leu, L-Phe) in the gas phase by a combined experimental and computational approach. Electrospray ionization-mass spectrometry suggested the formation of 1:1 anionic complexes between CDs and AAs and the complex anions were further identified by tandem mass spectrometry. Moreover, ion mobility-mass spectrometry experiments revealed the inclusion complexation adopted for $[\alpha\text{-CD+Gly}]^-$ as well as β-CD with either amino acid, whereas $[\alpha\text{-CD+Leu}]^-$ and $[\alpha\text{-CD+Phe}]^-$ favored an exclusion conformation, indicating size-dependent binding modes. The association is primarily driven by polar interactions via the formation of hydrogen bonds. Furthermore, the relative dynamic stabilities of the complex ions were observed to be in correlation with the gas-phase basicities of the deprotonated

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