

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

The Origin of “Magic-Number” Stability and Chiral Selectivity for Serine Clusters in Gas Phase ANTHONY COSTA, R. GRAHAM COOKS, Purdue University — Serine “magic-number” clusters have attracted substantial experimental and theoretical interest since their discovery. They have been implicated in one possible mechanism leading to the origin of homochirality, as certain clusters exhibit remarkable chiral selectivity. We aim to develop a “structural landscape” for these clusters over a range of relevant cluster sizes, enantiomeric compositions, and ionizing charge states using theoretical tools of statistical and quantum mechanics. In this work, we search for low-lying stationary points and global minima of the potential energy landscape via a combined annealing, replica exchange and basin-hopping molecular dynamics approach in a modified AMBER forcefield. These structures are used as inputs for further DFT-based optimization and energy decomposition analysis. It is shown that the behavior and stability of these systems is due to major structural rearrangements as a function of size and charge. Further, the experimentally observed chiral selectivity may be understood in part by the unique network of hydrogen bonds facilitated by the serine hydroxyl side chain. The influence of a further kinetic mechanism is not ruled out by the current results and is discussed.

Anthony Costa
Purdue University

Date submitted: 20 Nov 2009

Electronic form version 1.4