

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Simplified Hamiltonians for coarse-grained properties of large single-stranded RNA molecules PETER PRINSEN, ARON YOFFE, WILLIAM GELBART, Department of Chemistry and Biochemistry, UCLA — Large single-stranded RNA (ssRNA) molecules with a length of a few thousand to a few tens of thousands of nucleotides are quite common in nature. These RNAs generally have a highly branched secondary structure with many short, double-stranded sections. The secondary structure is important for function. However, the prediction of the thermally accessible secondary structures of large ssRNAs is complicated. There are several computer programs available that predict secondary structures of ssRNA. They produce good results for small molecules but are not very reliable for large ones. We are not interested in “high-resolution“ structures, however, but in more coarse-grained properties, for example the average three-dimensional size of the molecule. We expect that the available computer programs are useful for determination of these coarse-grained properties but the complicated Hamiltonians they use limit the usefulness of these models for further theoretical investigations. We show that one can simplify these Hamiltonians considerably and still retain important predictive power. The inclusion of stacking energies is crucial but many of the detailed energy rules are not. We define several measures for the size of a secondary structure and we show how these measures are related to each other.

Peter Prinsen
Department of Chemistry and Biochemistry, UCLA

Date submitted: 29 Nov 2007

Electronic form version 1.4