

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Semi-Classical Quantization of a [2] Rotaxane KARL SOHLBERG, ARI SILVER, Chem. Dept., Drexel University — Rotaxanes show tantalizing potential for functional nanosystems. A [2]rotaxane is a molecular complex consisting a long dumbbell-shaped chain molecule, (called the shaft) which threads a ring molecule, typically a crown-ether or cyclodextrin. The chain component is terminated on each end by a bulky substituent to prevent unthreading of the ring. The components are therefore chemically independent but mechanically interlocked. When such complexes are synthesized with two inter-component binding stations, bistability results, hinting at potential for switching or data storage applications. We have investigated the quantum-mechanical eigenstates associated with the shuttling motion between these co-conformations. The state density is very high because nano-systems exist at the transition/interface between molecular systems, which are dominated by quantum phenomena, and macroscopic systems where matter is essentially continuous and classical physics provides the best description. We show that state density is *highest* where quantum mechanical tunneling is most important.

Karl Sohlberg
Chem. Dept., Drexel University

Date submitted: 16 Jan 2006

Electronic form version 1.4