

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Semi-empirical Study of a Multi-associated Rotaxane KI-HO LEE, KARL SOHLBERG, Drexel University — Rotaxanes are prototype molecular devices based on two components; one or more ring molecules threaded by a dumbbell-shaped, shaft molecule. In a switchable rotaxane, the shaft has two or more sites strongly attracting the ring with different binding intensity, and translation of the ring between the sites may be induced by switching the relative binding intensity. For amine binding sites, for example, this switching may be accomplished by the protonation of the amine to form a cationic ammonium site. In this study, semi-empirical (AM1) electronic structure calculations have been carried out for a multi-ring, multi-shaft rotaxane. Each of three rings is threaded by a shaft and the three shafts are chemically bonded to each other, limiting the number of degrees of freedom in co-conformations of the entire complex. Each of the three shafts contains one bipyridinium site and one amine site. The latter can be switched to an ammonium site by protonation to induce translation of the associated shaft. We investigate concerted versus stepwise protonation of the amine sites.

Ki-Ho Lee
Drexel University

Date submitted: 30 Nov 2005

Electronic form version 1.4