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SUBSTITUTION CHEMISTRY OF THE HEXAMOLYBDATE ION: THE DEVELOPMENT OF REACTIONS FOR ROTAXANE PREPARATION

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Much interest has been generated lately in the synthesis of new materials to be used in the construction of molecular scale electronic devices and machinery. Rotaxanes have surfaced as potential building blocks for designing such structures. The simplest rotaxanes are dumbbell-shaped molecules consisting of a long chain linker unit threaded, non-covalently, through a ring-shaped unit and stoppered on each end with a large, bulky group. (Fig. 1) The object of this study is to synthesize a simple rotaxane, using various bifunctional organic molecules as the chain unit, a β-cyclodextrin molecule as the ring unit, and hexamolybdate ions as the stoppering groups. IR and 1H NMR analyses indicate that the hexamolybdate ion has been successfully synthesized from Na₂MoO₄ and (n-C₄H₉)₄NBr (Inorganic Syntheses). The main focus of this project is to explore the substitution reactions between the hexamolybdate ion and various aromatic amines, and, by analogy, to understand the chemistry of the substitution reactions between the hexamolybdate ion and the potential rotaxane linkers. There has been some preliminary success with the substitution of p-anisidine and 1,4-phenylenediamine onto the hexamolybdate ion, using high pressure sealed tube reactions at elevated temperatures. Analyses performed using 1H NMR and FAB-MS suggest that the aromatic molecules have been successfully substituted onto the hexamolybdate ion. (Fig. 2)