A summary of project results is reported.
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Final Report

by

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Macrocycles Containing Tin

The project involved the development of methods for the synthesis, purification and characterization of pre-organized macromolecular hosts containing several Lewis acidic tin atoms, and investigations of the potential for such compounds to bind anions and basic donors selectively. The rationale for the study was that macrocyclic species containing Lewis acidic sites should bind anions and donors within the cavity of the macrocycle in a manner analogous to cation binding by "crown ethers" and "cryptands", and that coordinatively saturated tin atoms, which can become pentacoordinate, are good candidates for the Lewis acids. Selective binding properties that correlate to the fit of an anion or donor in the organized binding region of the macromolecular host were expected, and such properties might be exploited for anion separation, anion identification, and catalysis.

A series of macrobicyclic hosts containing two Lewis acidic tin atoms as binding sites was developed, and anion binding was studied by $^{119}$Sn NMR spectroscopy (TR-1, Pub-2). Tricyclic, ditopic hosts containing four Lewis acidic tin atoms were developed (TR-2, Pub-3). X-ray crystal structure determinations of a number of the hosts were obtained (TR-4, TR-5, TR-6, TR-7, TR-8, TR-9, TR-10, TR-11, Pub-5). Solid complexes of macrobicyclic hosts binding anions were isolated and studied by X-ray crystallography and solid state $^{119}$Sn NMR spectroscopy (Pub-1). Force field parameters for compounds containing tetrahedral tin atoms were developed and evaluated (TR-3, TR-12, Pub-4). The structures of the macrobicyclic hosts were studied by molecular mechanics calculations, and the results were compared to the crystal structures (TR-13, Pub-5).
List of Technical Reports


4. "X-Ray Crystal Structure of 1,1,6,6,11,11,16,16-Octaphenyl-1,6,11,16-tetrasnannaeicosane", Martin Newcomb and John H. Horner, November 7, 1990

5. "X-Ray Crystal Structure of 1,7-Diphenyl-1,7-distannabicyclo[5.5.5]heptadecane", Martin Newcomb and John H. Horner, November 16, 1990


List of Publications:


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