

A ^1H NMR study on the complexation of tetraalkylammonium cations, mono and diprotonated amines, and amino acids with a derivatized cyclotetrachromotrolylene in an aqueous solution

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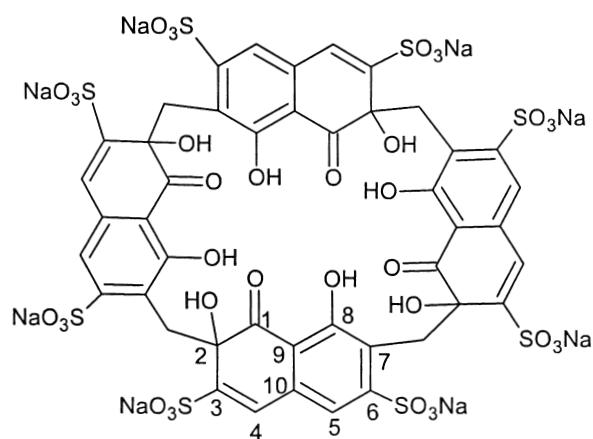
Abstract—The derivatized cyclotetrachromotrolylene host forms complexes of 1:1 host to guest stoichiometry with tetraalkylammonium cations and amino acids whereas complexes of 1:2 host to guest stoichiometry are formed with mono and diprotonated amines in an aqueous solution. Both electrostatic and hydrophobic interactions are involved in the complexation.
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1. Introduction

The study of host–guest complexation in an aqueous medium is of great importance because it provides an understanding of the chemistry in the biological system. Organic cations as guests have received extensive attention^{1–13} in the last decade, especially after the report that acetylcholine can be bound to acetylcholine esterase through interaction with aromatic residues present in the enzyme.¹⁴ Several reviews on the complexation of organic cations have also been published.^{15–19} Depending on the kind of host used, the non-covalent forces involved in the binding of the organic cations could be hydrogen bonding, π – π , CH– π , cation– π or cation–anion interactions. Until now only a few host molecules capable of binding organic cations in an aqueous medium have been reported and they are mainly from the sulfonatocalixarenes.

The water-soluble derivative of cyclotetrachromotrolylene (**1**) that we have synthesized recently, appeared to be a good host for organic cations. It has a rigid shallow bowl structure with exposed π surfaces for hydrophobic interaction and eight adjacent sulfonic anions on the upper rim for electrostatic interaction (CPK molecular models shown in

1a–1c). We were interested to gain an understanding of the interactions involved in the complexation of organic cations with **1**. This paper reports our study on the complexation of four tetraalkylammonium cations, four monoprotinated amines, three diprotonated amines and four amino acids with **1** in an aqueous medium at 25 °C using ^1H NMR spectroscopy.



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Keywords: Complexation; Stability constant; Tetraalkylammonium cations; Protonated amines; Amino acids; Derivatized cyclotetrachromotrolylene.

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