

Research Paper :

# Cucurbituril as a host molecule for the complexation of cations and acetamide in aqueous solution

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## ABSTRACT

Mixed ligand complexes of Cobalt and Nickel with acetamide and cucurbituril as host molecule were prepared and characterized using UV-Visible, IR and XRD techniques. These mixed ligand complexes are quite stable and this stability was largely attributed to the strong interaction of carbonyl oxygen donor atoms of cucurbituril with the cations. From the increase in absorbance in UV-Visible region the interaction between metal and host molecule was proved. The IR spectra showed significant variations, especially in  $3500\text{cm}^{-1}$  region and between  $1700$  and  $1200\text{cm}^{-1}$  indicating prevalence of enhanced hydrogen bonding. Cucurbituril cobalt benzamide complex showed two sharp peaks at  $2\theta = 31.7$  and  $25.89$ . This indicates that crystalline structure is still maintained in some complexes.

**Key words :** Cucurbituril, Host-guest complex, Supramolecular chemistry, Macrocylic molecule

The area of supramolecular chemistry has established itself as an emerging field in chemistry (Lehn, 1995; Vogtle, 1989; Balzani and De.Cola, 1992). Cucurbiturils (Fig. 1) are macrocyclic molecules consisting of glycouril repeat units. These compounds are particularly interesting to chemists because they are molecular containers that are capable of binding other molecules within their cavity. The name cucurbituril is derived from the resemblance of this molecule with the pumpkin of the family *Cucurbitaceae*. The cavity of Cucurbit[6]uril has nanoscale dimensions (Jason Lagona *et al.*, 2005) with an approximate height of 9.1pm, outer diameter 5.8pm and inner diameter 3.9 pm.

Cucurbituril is a rigid molecule and posses a hydrophobic cavity. At each entrance to the cavity, six polar carbonyl groups are located. These conditions are ideal for complexation of positively charged organic molecules with hydrophobic groups. So, the complexation of a large number of different ammonium ions by cucurbituril were studied first (Mock and Shih, 1983; Behrend *et al.*, 1905; Mock and Shih, 1988; Meschke *et al.*, 1997; Buschmann *et al.*, 1998a). Cucurbituril is also able to bind alkali and alkaline earth cations (Buschmann *et al.*, 1992; Hoffmann *et al.*, 1994; Buschmann *et al.*, 1998b). Cucurbituril is not soluble in many common solvents but it is found to be soluble in ionic and acidic solutions (Mock and Shih, 1986).

Host guest chemistry (Fig. 2) is the name given to the study of the encapsulation of one compound (the guest) by a second compound (the host) through non-covalent interactions. As a general rule, a host is chosen to be complementary to a particular guest such that in solution, a complex is formed spontaneously.

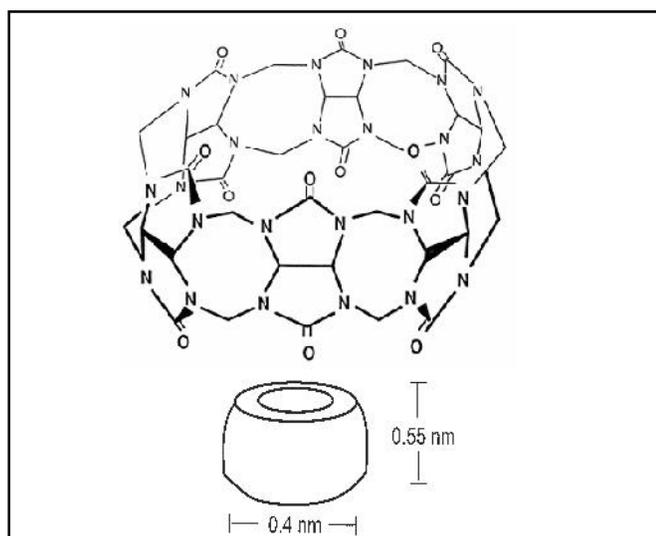


Fig. 1 : Structure of Cucurbituril

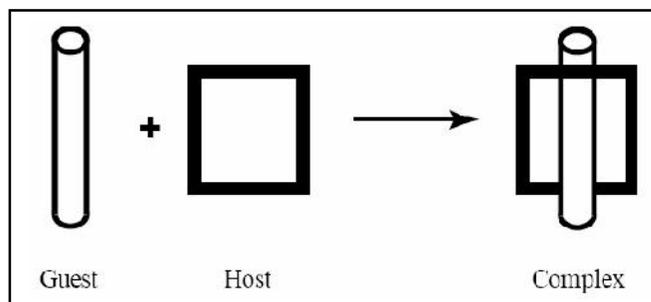


Fig. 2 : Host guest chemistry