Induced-circular dichroism resulting from the interaction between a chromophoric calix[6]arene and a chiral non-chromophoric amine

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Like resorcinarenes, cucurbiturils and cyclodextrins, calixarenes are supramolecular cyclooligomers. They are synthesized through the condensation of *p*-substituted phenols and formaldehyde. These macrocyclic molecules share a hydrophobic cage-like cavity (host) with the ability to complex a variety of organic derivatives (guests) such as cationic amines. They can be used as ion channel mimics, enzyme models, surface agents for protein recognition, or gene transfection vectors.

To study asymmetric host-guest interactions, we have used circular dichroism (CD) spectroscopy, and more specifically induced-circular dichroism (ICD). ICD is recorded when a non-chiral molecule interacts with a chiral molecule. Towards this aim, we have explored the effects of different parameters on the formation and the stability of an inclusion complex composed of a chiral amine, *i.e.*, (*S*)-(-)-2-methylbutylamine (chiral guest) and a calixarene, *i.e.*, [Zn.X_6tBu_6] (chromophoric host), where the small rim is functionalized by three imidazoles which are coordinated to a zinc atom. We have studied the effects mediated by amine concentration enhancement, solvents (dichloromethane and acetonitrile) and by temperature changes.

Whereas [Zn.X_6tBu_6], alone, exerts a negative Cotton effect with a negative maximum at 240 nm, a positive Cotton effect at the same wavelength is recorded when the complex is formed. Whereas the 1:1 complex is obtained with 1 eq. of (*S*)-(-)-2-methylbutylamine in DCM, it is formed in ACN with 5 eq. of the amine. Temperature effects show that the complex is more stable in DCM when compared to ACN. In conclusion, DCM appears as the most appropriate solvent to stabilize the complex resulting from [Zn.X_6tBu_6] and (*S*)-(-)-2-methylbutylamine.