

# Optical activity of the guest azobenzene molecule generated by inclusion complexation with steroidal bile acids

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Received 23 July 2004; accepted 30 August 2004

Available online 1 October 2004

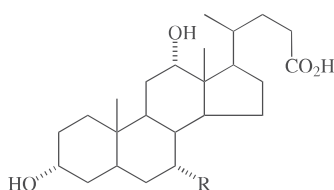
**Abstract**—The crystalline inclusion complexes of azobenzene **1** with cholic **CA** and deoxycholic **DCA** acid were prepared and their solid state CD spectra measured. The positive Cotton effect sign, corresponding to the lowest energy  $n-\pi^*$  transition, was correlated with the *M,M* helicity of the twisted guest molecule. The absolute sense of twist of the enclathrated guest molecule **1** was deduced from the X-ray structure of the **1-CA** complex. In addition, the solid state CD spectrum of the enantiomorphous crystals of methyl yellow **2** was measured. The source of the optical activity is a slight twisting of the constituent molecules and their helical arrangement in the crystal.

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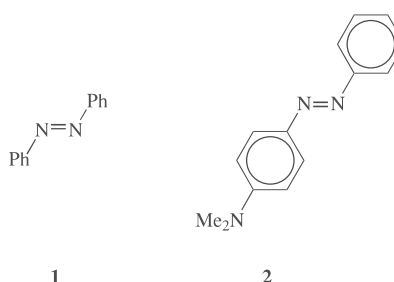
## 1. Introduction

Circular dichroism (CD) spectroscopy is a powerful tool in the determination of the molecular configuration and conformation in solution.<sup>1</sup> Unfortunately, its application is restricted to chiral compounds and the CD spectra cannot be measured for achiral molecules. However, optical activity can be induced into such systems by placing them in a dissymmetric environment.<sup>2</sup> Interaction of achiral molecules with chiral species in solution usually gives rise to an asymmetric perturbation of the chromophore or causes an excess population of rapidly interconverting enantiomers that leads to a measurable CD. In recent years, increasing

attention has been given to inclusion complexation of achiral guests with optically active hosts, like cyclodextrins or crown ethers.<sup>2,3</sup> The CD spectra of crystalline inclusion complexes appeared to be useful in the elucidation of the mechanisms of induction of optical activity particularly in combination with X-ray studies.<sup>4</sup> Owing to their ability to accommodate various types of organic substances within their crystal lattices, naturally occurring bile acids appeared to be very useful hosts for this purpose.<sup>5</sup> Recently, we have found that the molecules trapped in the cholic acid **CA** and deoxycholic acid **DCA** matrices are forced to assume chiral conformation that makes possible solid state CD measurements.<sup>6</sup>



CA, R = OH  
DCA, R = H



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