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Title: *Spectroscopic Determination of Binding Constants of Modified β-cyclodextrins with Brooker's Merocyanine*

Abstract:

Host-guest complexation occurs when a guest molecule is held inside a host molecule through weak molecular forces. β-cyclodextrin, a host molecule, has a variety of uses and is often applied in pharmaceuticals. Binding constants of host-guest complexes of Brooker's merocyanine and various modified β-cyclodextrins (2-hydroxypropyl-β-cyclodextrin, sulfated β-cyclodextrin, and methyl-β-cyclodextrin) were studied using fluorescence and UV-Vis spectrometry to determine the strength of interaction between the host molecule and the guest molecule. By modifying the β-cyclodextrin, the effect of ionic forces, hydrogen bonding, and steric hindrance were compared. It was determined via fluorescence spectrometry that sulfated β-cyclodextrin had a binding constant of 38.3 $M^{-1}$, which was significantly lower than the determined binding constants 430 $M^{-1}$ for β-cyclodextrin, 359.1 $M^{-1}$ for 2-hydroxypropyl-β-cyclodextrin, and 194.6 $M^{-1}$ for methyl-β-cyclodextrin. These results were confirmed via UV-Vis spectrometry, where the binding constants were 335.2 $M^{-1}$ for 2-hydroxypropyl-β-cyclodextrin

and 178.4 $M^{-1}$ for methyl-β-cyclodextrin. These results were in agreement with fluorescence data. The much lower binding constant of sulfated β-cyclodextrin could be caused by a combination of ionic forces and steric hindrance. A comparison of these results to the theoretical models will lead to verification of the effect of these forces on binding.

About the author:

Carly Hanson is a junior Chemistry major and German minor.