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A Theoretical Study of Brooker's Merocyanine with (2-Hydroxypropyl)-β-Cyclodextrin

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Title: *A Theoretical Study of Brooker's Merocyanine with (2-Hydroxypropyl)-β-Cyclodextrin*

Abstract:

To understand the important forces in host-guest complexes, a theoretical study of these systems was carried out using computational methods to better understand experimental results. β-cyclodextrin (BCD) is a cone shaped molecule where the narrow end is known as the primary rim and the wider end is known as the secondary rim. The host molecule being studied, (2-hydroxypropyl)-β-cyclodextrin (2HPBCD),is a modified version of BCD with hydroxypropyl (HP) groups substituted along the rims. Because this modification replaces some of the OH groups present in BCD, it removes their ability to hydrogen bond, while introducing new OH groups that are more flexible. This alters how hydrogen bonding can occur and the role it plays in 2HPBCD's complexations with Brooker's merocyanine (BM), which is a model conjugated dye molecule with oxygen at one end and a nitrogen group at the other end. The computational method used in the work was semi-empirical parametric method 3 (PM3) in Gaussian03 (G03). The PM3 optimizations were performed on many possible structures to determine the most stable structure. Results show that the most stable structure has the nitrogen end of BM at the primary rim, and doesn't appear to be positioned for proper hydrogen bonding.

About the author:
Ben is a senior chemistry major who grew up around computers. His father and brother both have computer science degrees. Combining an interest in computers and chemistry led to an interest in computational chemistry, which employs computers to answer relevant questions in chemistry.