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Review

Driving forces and electronic structure in β-cyclodextrin/3,3′-diaminodiphenylsulphone complex

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ABSTRACT

The complexation of 3,3′-diaminodiphenylsulphone (3DADPS) by β-cyclodextrin (β-CD) was analyzed using PM6 method and several combinations of ONIOM2 hybrid calculations in vacuum and in water. The objective was to elucidate electronic structure, driving forces and energy changes that accompany the complexation. Complexation and interaction energies, thermodynamic parameters, chemical reactivity and site selectivity of the molecular systems have been investigated. The results show that the inclusion process is exothermic. NBO calculations reveal that hydrogen bonding between β-CD and 3,3′-diaminodiphenylsulphone is a major factor contributing to the overall stability of the complex.

Contents

1. Introduction

β-Cyclodextrin (β-CD) is a cyclic oligosaccharide derived by enzymatic hydrolysis of common starch, which has an internal cavity shaped like a truncated cone of about 8 Å deep and 6.0–6.4 Å in diameter. This cavity possesses a relatively low polarity, so it can accommodate guest organic molecules inside [1]. Due to its particular chemical structure, β-CD can improve the stability, dispersing and dissolving properties of some drugs, and enhance its physical and chemical activity through the inclusion complexes [2]. Therefore, β-CD is by far the most widely used in pharmaceutical sciences and different fields of chemistry ranging from analytical to synthetic chemistry in CDs [3,4].

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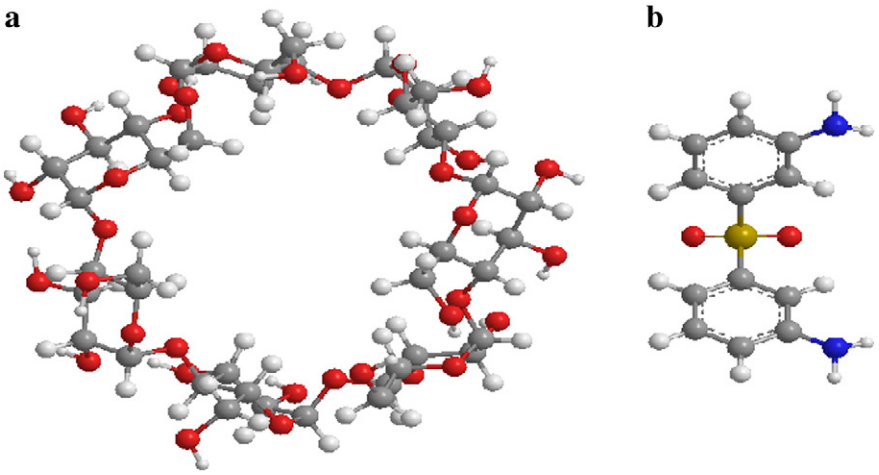

Fig. 1. Geometrical structures of β-CD (a) and 3DADPS (b) optimized by PM6 method.

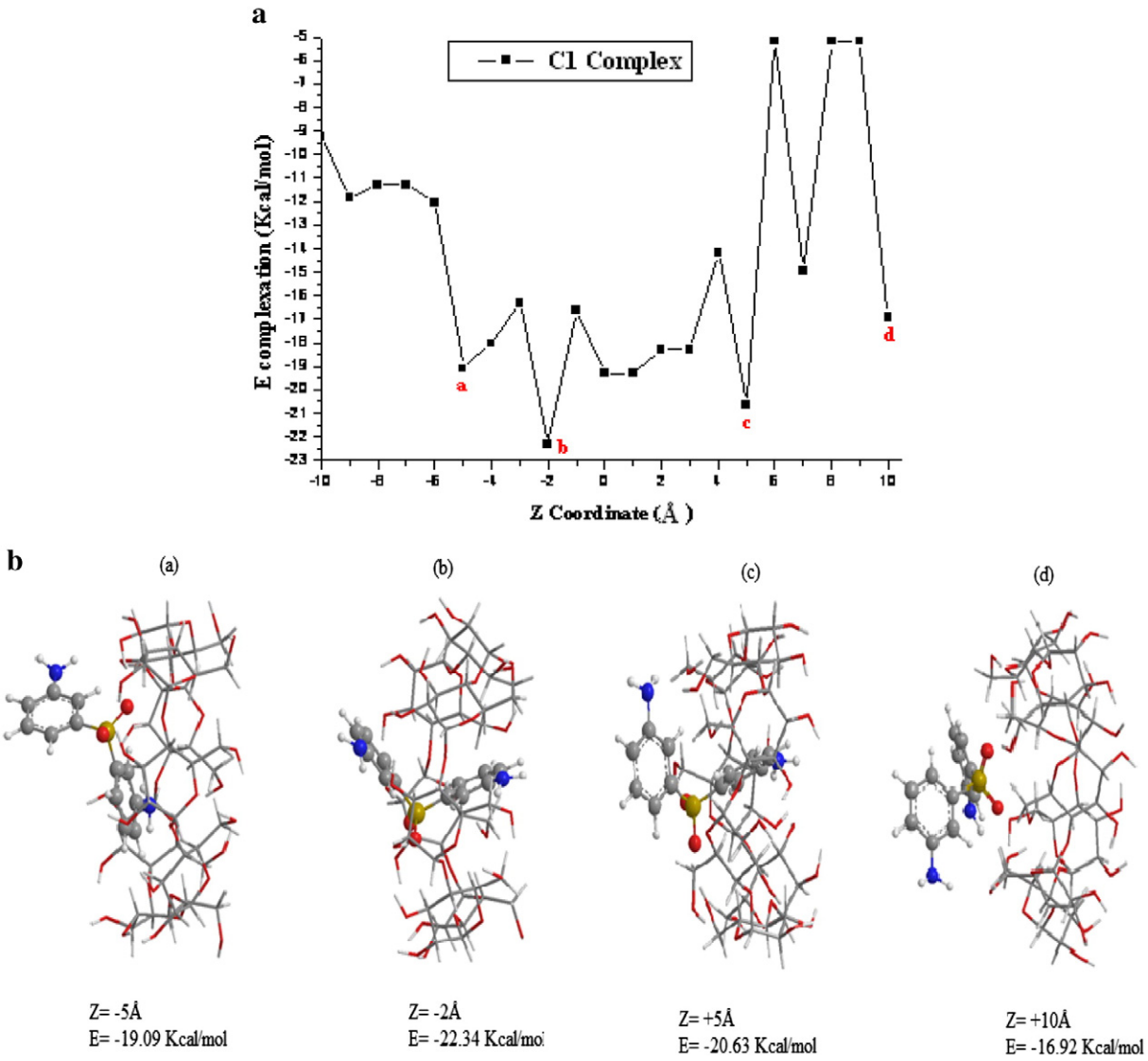

Fig. 2. Evolution of the complexation energy (a) and the optimized molecular geometry (b) during the movement along the Z axis of the inclusion complexation of 3DADPS into β-CD, PM6 calculations.