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Theoretical study of the hydration structure and interaction energy of Sorbitan monostearate (Span60) by using hybrid quantum mechanical/molecular mechanical (QM/MM) method

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The hybrid quantum mechanical/molecular mechanical (QM/MM) method has been used to investigate on mono-hydration and poly-hydration phenomena of the polar head group of Span 60 molecule in both gas and aqueous phases. Our calculations were performed by using Gaussian 09 program. The result indicates that Span 60 interacting with one water molecule shows the mono-hydration effect of the head group. When adding more water molecules around the Span 60 head group, the poly-hydration phenomena is clearly observed. Thus, it suggests that the QM/MM approach in this work is the precise and efficient method to investigate on the conformation and the hydration structure as well as the interaction energy of the Span 60 polar head group.

Keywords: Span 60, QM/MM method, hydration structure and interaction energy

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