

# A DFT study of infrared spectrum of sphingomyelin lipid molecule with calcium cation

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One of the phospholipid, sphingomyelin (SM) is the most abundant component of mammalian membranes in the brain and nervous tissues. The role is important for apoptosis, aging, signal transduction with cations. Recently, M.C. Yappert and co-researchers have shown that human lens sphingomyelin and the hydrated derivative, dihydrosphingomyelin (DHSM) are interacted with  $\text{Ca}^{2+}$  ions to develop human cataracts [1, 2].

In this study, we investigate conformational differences between an isolated SM/DHSM molecule and  $\text{Ca}^{2+}$ -coordinated form by means of DFT calculations. B3LYP adiabatic connection functional and 6-31G(d,p) split-valence basis set is applied according to the line of previous approaches in the phosphate group and metal cations interaction [3, 4].

As a result of geometry optimization and normal mode analysis, calculated infrared spectrums are obtained. The resultant conformations of SMs have hydrogen bonding in the different positions, OH group with phosphate group and with amide group, respectively. The red shift of amide band due to  $\text{Ca}^{2+}$  is compared with experimental infrared spectrum. Finally, we discuss the  $\text{Ca}^{2+}$ -induced changes from conformational and spectroscopic viewpoint to compare the experimental conclusions.

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