Characterization of the structure of PDP-DPPC bilayers by DFT and PM3 calculations.

Autorzy

Katarzyna Cieślik-Boczula

Aleksander Koll

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Streszczenie

The character of 3-pentadecylphenol (PDP)-dipalmitoylophosphatidylcholine (DPPC) interactions in a bilayer system was investigated using DFT and semi-empirical calculations. The obtained results were supported by ATR-IR spectra. The strongest intermolecular hydrogen bond was found between the phenolic OH and the PO2 groups of the DPPC molecule. The presence of water and hydrocarbon chains slightly weakens the strength of this PDP-DPPC interaction. In contrast to a pureDPPC bilayer, thewater molecules do not destroy the H-bonds formed by PO2 moieties and even enhance the total energy of the interaction. Both the van derWaals'interactions in the hydrophobic core of the PDP-DPPC aggregate and the intermolecular H-bond in the hydrophilic part make this complex more rigid, which influences its physical and chemical properties.

Słowa kluczowe

phendic lipid, doped DPPC bilayer structure, ATR-IR spectra, molecular interaction