Experimental report

24/05/2022

Proposal: CRG-2728 **Council:** 10/2019

Title: Understanding the high-temperaturemolecular motion of a model protomembrane architecture

Research area:

This proposal is a new proposal

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Samples: Decanoic acid: Decanol 1:1 + 2% perdeuterated eicosane (/squalene)

Instrument	Requested days	Allocated days	From	To
IN6-SHARP	4	4	14/08/2020	17/08/2020

Abstract:

Exp. Report CRG-2728

Understanding the high-temperature molecular motion of a model protomembrane architecture

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Modern phospholipid membranes are known to be in a functional, physiological state, corresponding to the liquid crystalline phase, only under very precise external conditions. The phase is characterized by specific lipid motions, which seem mandatory to permit sufficient flexibility and stability for the membrane. It can be assumed that similar principles hold for proto-membranes at the origin of life although they were likely composed of simpler, single chain fatty acids and alcohols. In the present study we investigated molecular motions of four types of model membranes to shed light on the variations of dynamics and structure from low to high temperature as protocells might have existed close to hot vents.

As proto-cells or proto-membranes are no longer accessible due to evolution, the only way to probe the properties of these hypothetical systems is to re-construct membranes from simple lipids with short chain lengths, presumably favored by prebiotic synthesis, and to expose them to the supposed environmental conditions. Here we concentrate on fatty acids, fatty alcohols and phospholipids, all with chain lengths of 10 carbons (named hereafter C10), which are among the shortest to self-assemble into lipid bilayers (see figure 1).

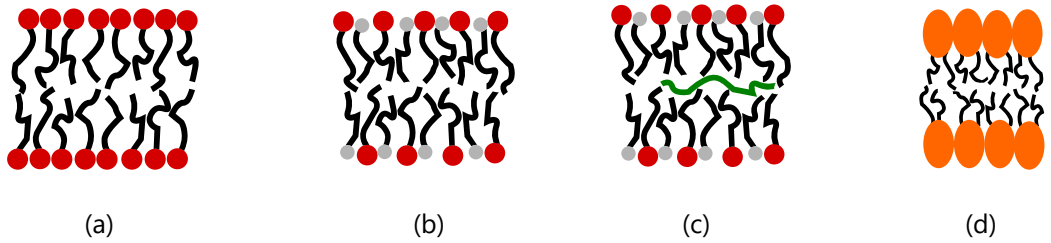

Figure 1: Four models for protomembranes: (a) Capric acid, (b) Capric acid + decanol (C10mix), (c) C10mix + eicosane, (d) DCPC.

To characterize their molecular dynamics, we performed elastic incoherent neutron scattering (EINS) and quasi-elastic neutron scattering (QENS) studies on the instrument IN6-SHARP with an energy resolution of 70 μeV in the temperature range from 278 to 355 K. The EINS measurements were done continuously with a temperature step of 1 K and a measuring time of 2 minutes per point. QENS measurements were conducted on the same samples at the temperature points of 278, 293, 323 and 353 K for 2.5 hours each. Additionally, the bicine buffer was measured in the same conditions with the exception that the QENS scans were acquired for only 2 hours due to time limitations. An empty cell and the completely incoherent scatterer vanadium were measured at room temperature for correction and normalization purposes.

The EINS data were analysed in terms of the Gaussian approximation and atomic mean square displacements (MSD) were extracted [1] (see figure 2). All samples presented very similar slopes, e.g. stabilities against temperature, and a clear hierarchy in flexibility.

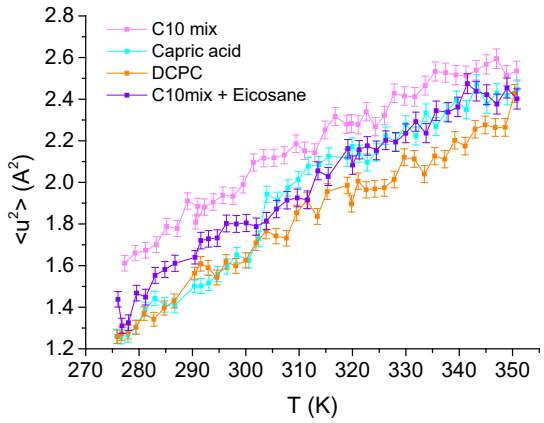

Figure 2: MSD for the four samples as a function of temperature.

We further analysed the QENS spectra (see figure 3) and were able to distinguish three different kind of motions: translational diffusion, jump diffusion and small vibrations.

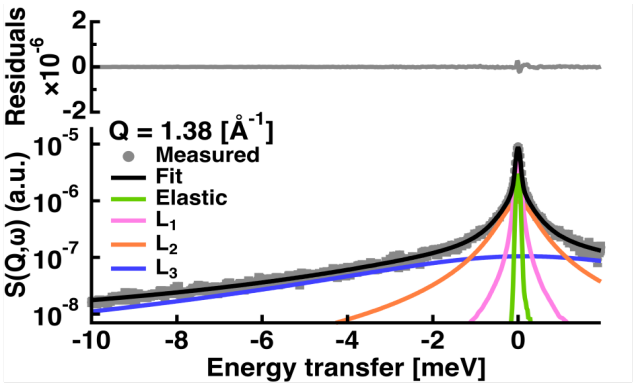

Figure 3: Example of fit results for the spectrum of capric acid at Q = 1.38 Å^{-1} and T = 293 K.

We further applied the Matryoshka model [2-4], which was recently developed by our group to describe molecular motions in lipidic membrane samples, to get more detailed information about the differences in the dynamics of the four samples. The results of the data analysis were now submitted to the Journal Phys. Chem. Chem. Phys.

References:

1. Rahman, A., K.S. Singwi, and A. Sjolander, *Theory of Slow Neutron Scattering by Liquids .1.* Physical Review, 1962. **126**(3): p. 986-996.
2. Bicout, D.J., et al., *The dynamical Matryoshka model: 1. Incoherent neutron scattering functions for lipid dynamics in bilayers.* BBA - Biomembranes, 2022. **1864**: p. 183944, 1 - 19.
3. Cisse, A., et al., *The dynamical Matryoshka model: 2. Modeling of local lipid dynamics at the sub-*

nanosecond timescale in phospholipid membranes. BBA - Biomembranes, 2022. **1864**: p. 183950.

4. Matsuo, T., et al., *The dynamical Matryoshka model: 3. Diffusive nature of the atomic motions contained in the Matryoshka-model for deciphering local lipid dynamics.* BBA - Biomembranes, 2022. **1864**: p. 183949.