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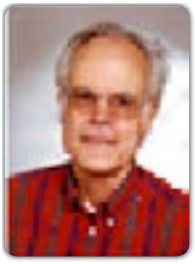

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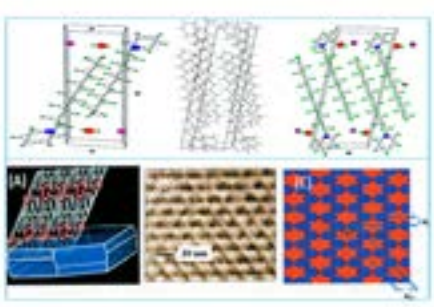
Crystal structures of synthetic and natural surfactants: topology and polymorphism

Synthetic surfactants are classified according to their polar groups in cationic, anionic and non-ionic entities. Biologically active surfactants from microorganisms are amphiphilic compounds where the polar part is built from e.g. long chain fatty-, chiral hydroxy fatty- or n-alkyl- -hydroxy fatty acids 1 . The polar part can be a phosphorylated carbohydrate as noticed in lipid A phosphates, the abundant component of bacterial lipopolysaccharides (LPS) and found on the surface of Gram-negative bacteria outer membrane, effecting the mucosal and systemic immunity, playing a potential role for microbial keystone species in autoimmunity, and in cancer chemotherapy 2 . Cyclic decapeptides e.g. the antibiotic tyrocidines are among the ones with a peptide backbone and the ornithine lipids. Synthetic N-cationic surfactants including those of the benzethonium type gained new interest due to their antiviral properties at submicellar concentrations, M 3-5 . Notably, the crystal structures vary with the counterions e.g. chloride, bromide, or with chiral anions i.e. S or R lactate or (2R,3R)-tartrate. However, non-spherical lipid A-phosphate and approximants self-assembled to form body-centered and face-centered cubic 2-d liquid crystals 6 ; for lipid A-monophosphate, rhombodo-decadecahedra (Fd3m) packing is suppressed because of instability in the mean curvature between the tetrahedral and the octahedral nodes. Tetrakaidodecahedra packing showed only tetrahedral nodes; the tetrahedral angle could only be retained between all edges if the hexagonal faces of the truncated octahedron were changed 7 . The quasicrystals exhibited non-crystallographic packing of non-identical lipid A-phosphate spheres 8 . The spatial packing of these spheres was in either a cuboctahedron or an icosahedron. It was noted that the observed (3.3.4.3.4) was a crystalline analogue of the icosahedral quasicrystal. The tiling pattern of triangles (N3) and squares (N4) possessed a p4gm plane group. Another coded lipid A-diphosphate approximant showed an 8/3 ratio, with 6-fold symmetry and plane group p6mm. Both and dodecagonal phases revealed a N3/N4 ratio of approximately 2.34. Because of bond-orientational order the direction of domains was classified into three orientations for the (3.3.4.3.4) tiling, but only two for the 8/3 approximants.



of lipid A-diphosphate; (B) HRTEM image of antagonistic lipid A-diphosphate; (C) schematic tiling structure of lipid A-diphosphate corresponding to the HRTEM image shown in (B).

Biography

Prof. Henrich H. Paradies, FRSC & CC, MD, Ph.D., Ph.D., D.Sc. (h.c.), MinstP, studied bioinspired, smart and multi-scale materials with defined wettabilities of cationic lipids as components in antiviral, antibacterial, and anti-inflammatory ingredients, the inhibition of viral activities on the level of monomer or cluster sizes (cyclic peptides), adherence for brushy surfaces by clinging to flaws and function of the organization on their specific head groups e.g. ammonium vs. phosphonium groups, Zn-cationic lipid-alendronate complexes or cyclic peptides with antimicrobial activities. The uptake of these materials is dependent on free diffusion, micelle endocytosis, distribution through the cytoplasms and disassembles into monomer to unfold full biological activities. A unique role plays the lipid A-phosphates and their approximants as antagonist for chronic inflammation, food poisoning, allergens and resistance against antibiotics. The mechanics and physics of these supramolecular assemblies were analyzed in terms of bond-orientational order, mean field phase diagram and disproportionate crystals or quasicrystals. (orcid.org/0001-0003-9409-3471).

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