Theoretical study of the interaction beetwen an organic tubular structure and the Na^+ ion

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Several classes of organic tubular structures are known, made up by self-assembling of macrocyclic units [1]; among these, the hollow tubular systems set up by stacking of cyclopeptides derived from alternating D- and L- -aminoacids can be utilised as suitable devices for building intermembrane ion channels with performances comparable to that of their natural counterparts [2]. In fact, the side groups of the aminoacids can be chosen so as the resulting tubular structure can be inserted inside a lipidic double layer [3].

In the framework of the computational study on tubular systems undertaken by our research group [4], we attempted to study, by using accurate quantum-mechanical methods, the interaction between a cyclopeptidic tubular system and a positive ion (Na+) inside its cavity, so as to give some insight in the transport process of a cation through a tubular system.

References:
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