Molecular Recognition of Adenine, Adenosine and ATP at the Air-Water Interface by a Fullerene-Uracil Adduct

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Molecular recognition of adenine, adenosine or adenosine 5'-triphosphate (ATP) at the air-water interface by an uracil-appended [60]fullerene, C_{60}, was studied by using the Langmuir and Langmuir-Blodgett techniques. For that purpose, C_{60} was derivatized to bear an uracil base, i.e., 2-(5'-uracil)fulleropyrrolidine (**1**) was prepared. This newly synthesized fullerene adduct was characterized by ESI-MS as well as the UV-visible, IR, NMR spectroscopy and electrochemistry techniques. The molecular recognition driven base-pairing between C_{60}-uracil and adenine, adenosine or ATP, modeled by using *ab initio* B3LYP/3-21G(*) calculation methods, revealed the Watson-Crick type base-pairing. The isotherms of surface pressure versus area per molecule for the Langmuir films of **1** were obtained and values of compressibility of the films determined. Addition of a conjugate base, such as adenine, adenosine or ATP to the water subphase stabilized the monolayer film of **1** and increased the limiting area per molecule extrapolated to the zero surface pressure, A_1, from 2.2 ± 0.1 nm^2 for water subphase in the absence of the base to 3.1 ± 0.2 for ATP present in the subphase. The determined A_1 values are close to those theoretically estimated for the base-paired conjugates at horizontal orientation in the monolayer films. The Langmuir-Blodgett films of **1** were characterized by electrochemical methods. The Brewster angle microscopy images of films of **1** revealed different aggregation properties in the presence and absence of the conjugate bases in the water subphases.