

# Hydrophobic Hydrating of the Polycyclic Aromatic Hydrocarbon (PAH) Anthracene in Amorphous Ice

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Polycyclic aromatic hydrocarbons (PAHs) constitute a class of carbon and hydrogen compounds characterized by the presence of two or more benzene rings, either individually or fused together within their molecular structure. These compounds, known for their limited solubility in water, can undergo photo-oxidation and degradation to simpler substances. In this study, we focused on anthracene ( $C_{14}H_{10}$ ), a typical PAH, given its significance in medicinal applications. Anthracene derivatives have demonstrated promising potential as effective anti-cancer agents. We investigated the molecular organization of anthracene around water using Molecular Dynamics (MD) computational technique. The relevant of this work ascertain what role the water plays in the solubility in anthracene and can guide future investigations of drug solubility in polycyclic aromatic hydrocarbons: a major issue to design bioavailable drugs.