Understanding the aggregation mechanism and stability of asphaltenes

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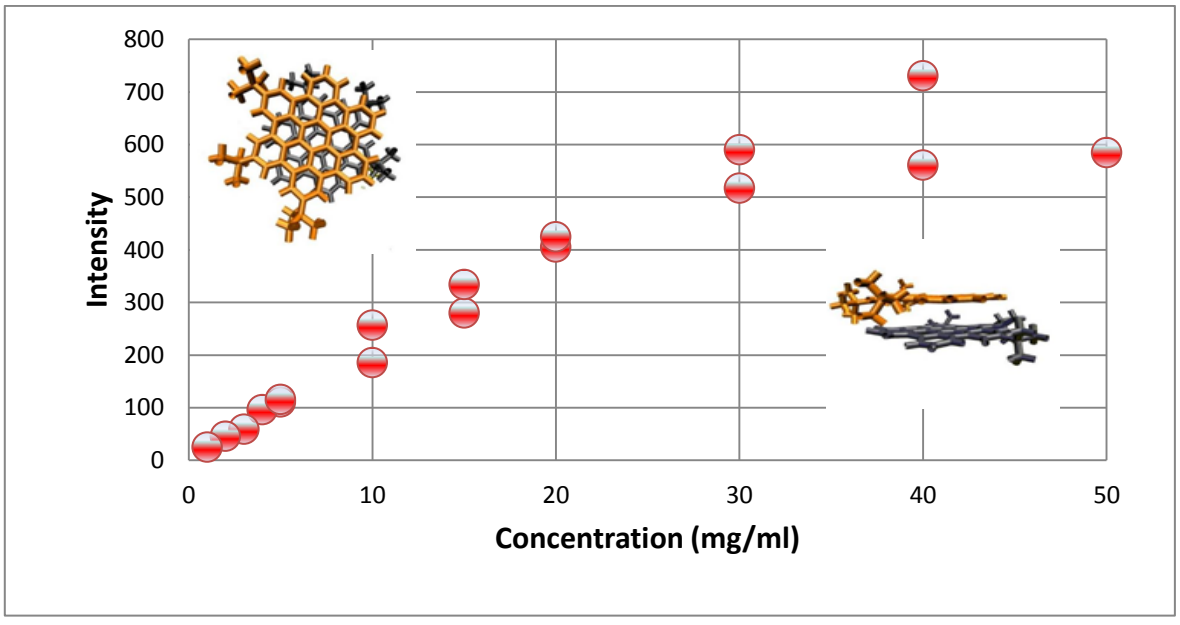
Asphaltenes, a class of aromatic compounds within crude oil, pose significant industrial challenges such as reservoir impairment, inefficient separation of water from oil, and obstruction of pipelines. Because natural asphaltenes possess an undefined molecular structure which results in a complex aggregation mechanism, a model compound, hexa-*tert*-butyl-hexa-*peri*-hexabenzocoronene (HTBHTC) was studied in toluene and heptane, in order to understand the behaviour of natural asphaltenes.

The kinetics of the colloidal system are examined as a function of time and concentration by an intensity based light scattering approach, while the molecular interactions were investigated by molecular dynamic simulations.

The intensity of the light scattered by the HTBHTC was measured over a period 366 hours, so that the aggregation kinetics of the polyaromatic compound are established. The intensity was found to be linear to the HTBHTC concentration, while the addition of heptane did not affect the stability of the already formed aggregates. Molecular dynamic simulation results are consistent with the experimental conclusions.



Intensity as a function of concentration and the stacking of HTBHTC molecules

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