Self-assembly of anionic boron cluster compounds

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Solution behavior of decaborate, dodecaborate, 1-carba-dodecaborate, mercaptododecaborate and cobalt bis(1,2-dicarbollide) anions was extensively studied by NMR spectroscopy, conductivity, tensiometry, cryoTEM and SAXS. All the experiments indicate that the boron clusters form multimolecular aggregates in solution and are surface active despite an absence of a hydrophobic tail as compared to classical surfactants. The studied compounds comprise the boron clusters of various hydrophile-lipophile balances: from small and hydrophilic decaborate with high charge density (resembling thus hydrotropes) to bulky and hydrophobic metallacarborane (behaving like surfactants). The series can be divided into two groups: (i) bulky metallacarborane with a prolonged molecule, the aggregation of which is enthalpy driven and obeys the mechanism of the closed association with small aggregation number and no condensed counterions [1]. (ii) Small and highly symmetric *closo*-(carb)boranes with relatively high aggregation number without an electrostatic restriction due to the effective counterion condensation. The aggregation takes place regardless of the exoskeletal substitution (BSH) or the presence of C-H units within the cluster. The driving force for all above-mentioned processes is closely related with a hydrophobic effect.



Figure 1 Self-assembly of anionic boron cluster compounds.

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[1] M. Uchman, V. Dordovic, Z. Tosner and P. Matejicek, Angew. Chem. Int. Ed., 2015, 54, 14113.