The Rational Design of Molecules for Use as Friction Modifiers

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Car engines require protection from corrosion and wear. To this end it is possible to attach small molecules to the metal surfaces which can form a layer and reduce friction and corrosion. Previous work has shown that carboxylates are good head groups for attachment of molecules to metallic surfaces containing iron [1].

We have been looking at the binding of carboxylate molecules to lightly oxidised Fe(III) systems through statistical trends in similar systems present in the CSD. We are interested in the geometry of these systems to enable us to understand what makes the carboxylate group a good surface active group for such systems. From this we hope to be able to design molecules which can attach to iron surfaces in a controlled, predictable way in order to function as friction modifiers.

Thus far we have shown that of all the common binding modes, the binding of each oxygen atom in the carboxylate to two different iron centres is the most prevalent form. On closer inspection there appears to be little strain in the bond angles of the carboxylate and only minor distortion of the iron centres from regular octahedral geometry. This suggests that there is good orbital line-up between the two moieties and is thus it is a good template for the design of an attachment group.

[1] Harris S.G., *University of Edinburgh,* 1999.

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