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Modeling the chemistry of hydrotreating; the hydrodesulfurization, hydrodenitrogenation, hydrodeoxygenation and hydrodemetallation of fossil fuels

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Although chemistry may be viewed as a maturing discipline of science and the chemical industry seems now to hold a secure but not rapidly growing sector of the economic marketplace, there is, in fact, a revolution in progress. The rate of change in the manner in which we do chemistry has never been greater. Within the academic environment the last decade has been witness to the invasion of computers into the laboratory and to the ever more sophisticated and rapid methods of analysis and characterization. Within industry many of the bulk commodities remain the same but their methods of production are continually changing. This change is driven by two factors. First, the old factor that has always been present in the marketplace, the continuing need to obtain a competitive edge in the economy of production. Second, and this will become increasingly important as the world becomes a global village for a seemingly ever increasing population with higher demands for energy and advanced technologies, the drive for chemically benign processes [1]. This is sometimes referred to as the "greening of chemistry" [2]. The search is on for syntheses that show atom economy and avoid the problems associated with undesirable by-products. There is a search for reactions that may be carried out in water, supercritical carbon dioxide or some similar ecologically friendly medium which avoids the use of organic solvents. Being mindful of our environment is, indeed, a global concern and is one that is at the heart of hydrotreating of fossil fuels. The controlled removal of sulfur, hydrodesulfurization, DHS, and hydrodenitrogenation, HDN, form the basis for the elimination of SO_x and NO_x emission in the burning of oil, gasoline and all refined petroleums. The removal of oxygen from fossil fuels is unnecessary given that certain oxygenates are used as additives to increase octane ratings in automobile petroleums, However, the process of hydrodeoxygenation, HDO, is competitive with HDS and HDN and so consumes hydrogen gas thereby adding to the overall expense of hydrotreating. The presence of metal ions in heavy crude oils, the so-called bottom of the barrel, is deleterious because the metal ions once released affect catalytic performance in a negative fashion. The actual mechanisms, the detailed chemical reaction pathways of the hydrotreating processes are not known. Thus academic curiosity has led to the development of an academic cottage industry. Surface scientists, chemical engineers, organometallic chemists and theoreticians have been attracted to the study of how sulfur, nitrogen, oxygen and metals are removed from the organic molecules present in fossil fuels that contain these elements. In this Symposium-in-Print, key workers in this field express their views and summarize their results.

REFERENCES

1. *Financial Times* Survey: The Chemical Industry. 26 September 1996.
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