

# Lawrence Berkeley National Laboratory

## Recent Work

### Title

PROGRESS REPORT FOR OCTOBER AND NOVEMBER 1980 - METAL COORDINATION CHEMISTRY: RECOVERY AND REMOVAL OF METAL FROM HEAVY CRUDE AND SHALE OILS WITH MULTIDENTATE LIGANDS

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November 26, 1980

TO: Dexter Sutterfield, BETC

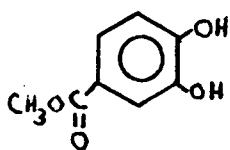
FROM: R. H. Fish and T. Vermeulen

SUBJECT: Progress Report for October and November 1980  
Metal Coordination Chemistry: Recovery and Removal of Metal from  
Heavy Crude and Shale Oils with Multidentate Ligands

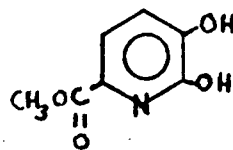
## METAL COORDINATION COMPOUNDS OF ARSENIC

Previously we identified several inorganic arsenic and organoarsenic compounds in oil shale retorting products that either emanate from a biogeochemical origin or were formed in the retorting process<sup>1</sup>. Because of the known role of arsenic species in poisoning catalysts used in subsequent refining processes, we have directed our efforts toward finding new chelating agents to react with these identified inorganic arsenic and organoarsenic compounds.

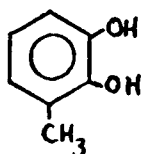
In this regard, we have started our metal coordination chemistry project by reacting the compounds we have speciated, namely arsenate ( $\text{AsO}_4^{3-}$ , 1) and methyl- and phenylarsonic acids ( $\text{MeAs}(\text{OH})_2$ , 2;  $\text{C}_6\text{H}_5\text{As}(\text{OH})_2$ , 3) with multidentate ligands 4-7:



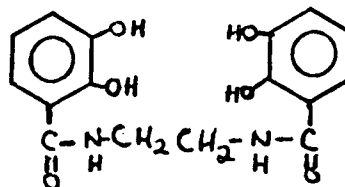
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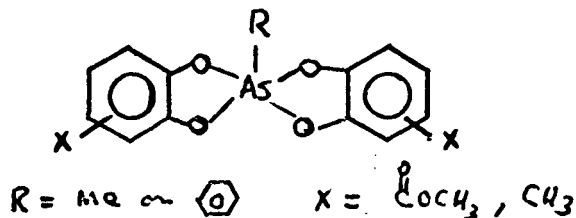


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The following type of five coordinate arsenic complexes were isolated for arsenic compounds 2 and 3 with ligands 4-7:



These were identified by nuclear magnetic resonance spectrometry (250 MHz) and electron-impact mass spectroscopy. We are continuing these studies with other multidentate complexes that have the potential to be placed in a polymeric backbone.

#### SPECIATION STUDY ON HEAVY CRUDE AND SHALE OILS, SOLVENT-REFINED COALS, AND DONOR-SOLVENT COAL LIQUIDS

Eight samples from BETC of synthetic and crude oils are to be analyzed for compounds containing arsenic, vanadium, nickel, and possibly other metals. This will be accomplished by use of a high-performance liquid chromatograph coupled with a graphite-furnace atomic-absorption spectrometer as the element-specific detector. A preliminary analysis of total metal content by x-ray fluorescence spectrometry is being carried out by Robert Giaouque of LBL, results of which will be reported in the first quarterly report.

#### REFERENCES

1. R. H. Fish, J. P. Fox, F. E. Brinckman and K. L. Jewett, Science (1980). Submitted.

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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