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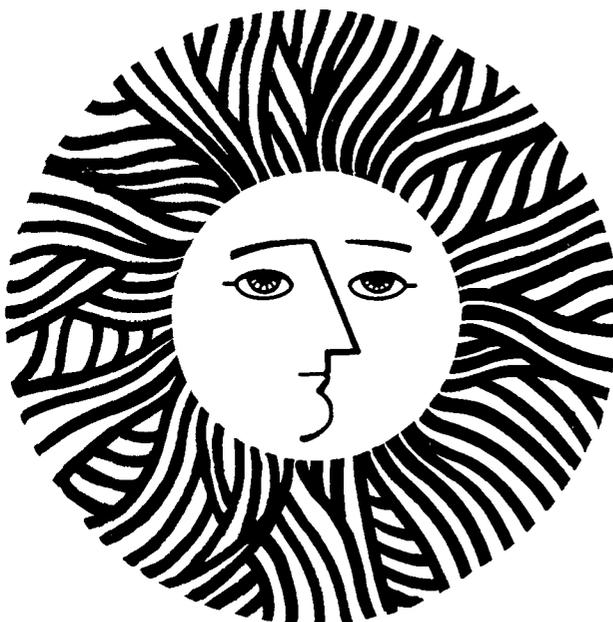
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March 10, 1980

TO: Art Hartstein

FROM: Bob Giaugue, Richard Fish, and Phyllis Fox

RE: February Monthly Progress Report
The Partitioning of Major, Minor, and Trace Elements
During Simulated In-Situ Oil Shale Retorting
LBID-178

NAVY CORE PROJECT

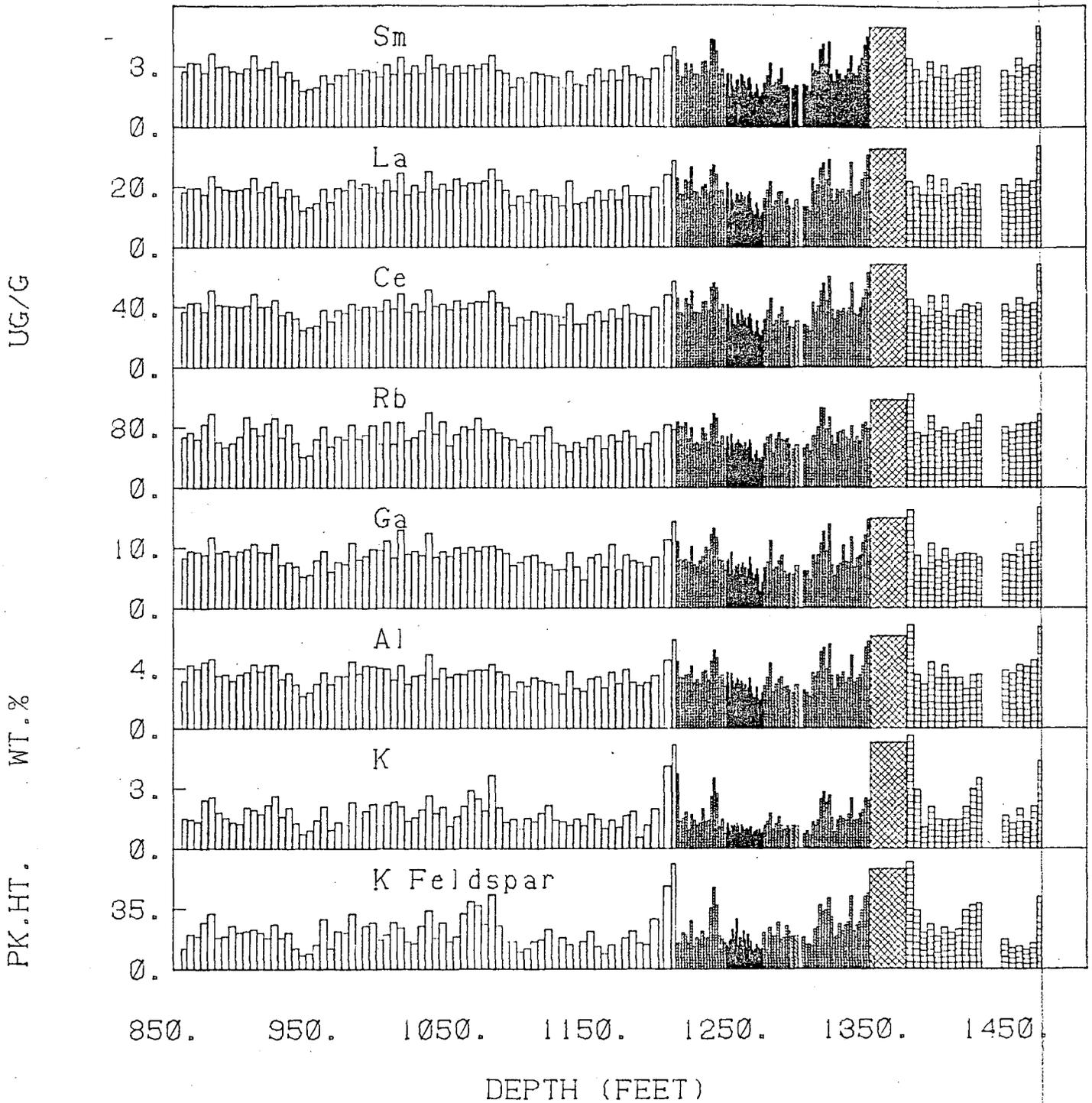
Data Analysis

The data base for Core 15/16 was completed with the receipt of the analyses of nitrogen, hydrogen, organic carbon, and inorganic carbon from LETC. Pearson correlation coefficients and statistical significance values were computed for Core 15/16 incorporating the modified procedures described in the January Monthly Progress Report. Depth histograms of elemental and mineral concentrations were plotted; typical histograms are shown in Figures 1 and 2.

Data quality control analyses were initiated. A number of calculation procedures were developed to verify the accuracy of the data. These included calculating the ratio of the sum of the nitrogen, hydrogen, and organic carbon to the oil weight and conversion of independent elemental analyses by neutron activation to respective mineral phases and comparison with X-ray diffraction data. The correlations and histograms were also inspected in order to identify spurious results. These analyses and comparisons led to the identification of several spurious data points and work was initiated in order to resolve the discrepancies by reanalysis or verification of original calculations.

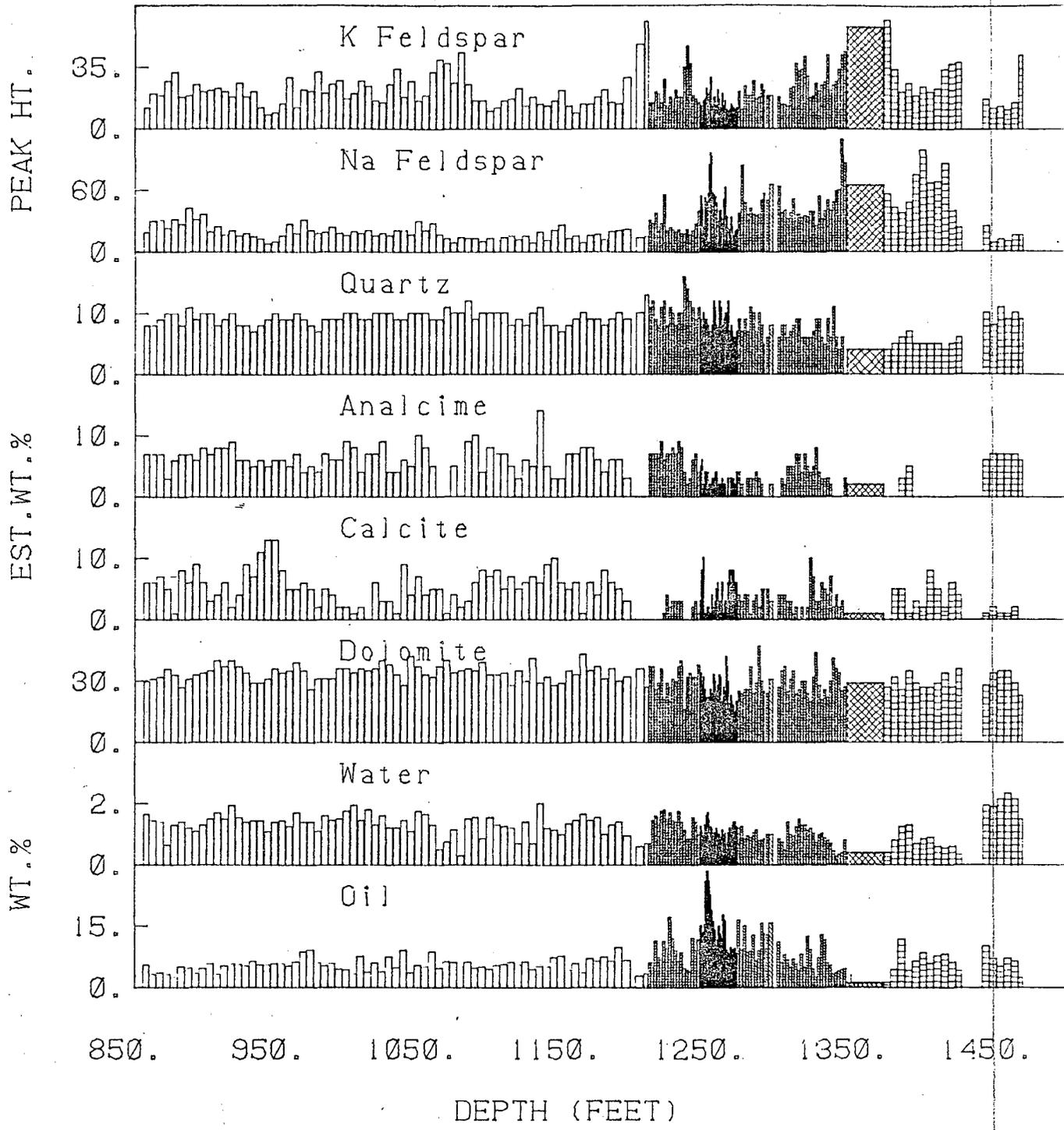
Cadmium Measurements

The cadmium analyses of core hole 25 were completed in triplicate. These analyses indicate that cadmium in this core ranges from 0.22 to 1.42 mg/l.



CORE HOLE 15/16

Figure 1. Histogram of seven elements and Potassium Feldspar in core hold 15/16.



CORE HOLE 15/16

Figure 2. Histogram of six minerals and Fischer-Assay of oil and water results in core hole 15/16.

IDENTIFICATION AND QUANTIFICATION OF FATTY ACIDS AS LIGANDS OF METALS IN OIL SHALE PROCESS WATERS

Previously, we reported the completion of fatty acid profiles for seven oil shale process waters. This month, we extended this work to include the quantification of normal and branched fatty acid methyl esters previously identified by GC-MS. The concentration of fatty acid methyl esters in the benzene fraction of Occidental's boiler blowdown water are shown in Table 1.

IDENTIFICATION OF NITROGEN ALIPHATIC AND AROMATIC HETEROCYCLIC COMPOUNDS AS LIGANDS OF METALS IN OIL SHALE PROCESS WATERS

In November 1979, we reported that there were nitrogen aliphatic and aromatic heterocyclic compounds present in Occidental's heater treater water. This work was continued this month in order to identify and profile nitrogen aliphatic and aromatic heterocyclic compounds in other process waters.

Samples of 150-ton and Geokinetics retort water were extracted with methylene chloride (pH^v9). The methylene chloride extracts were concentrated and placed on a dry florisol column and eluted under gradient conditions (100 percent hexane to 100 percent methylene chloride to 100 percent isopropyl alcohol). The fractions that had absorptions at 254 nm (UV detector) were analyzed by capillary column gas chromatography. Identification of the initial compounds, eluted with hexane methylene chloride, by capillary column gas chromatography-quadrupole mass spectrometry indicated the presence of methyl substituted phenols in Geokinetics' retort water.

Thus a new series of ligands that could complex metals associated with the process waters has been identified. We are presently analyzing the remaining fractions for nitrogen aliphatic and aromatic heterocyclic compounds in both Geokinetics and 150-ton retort waters.

Table 1. Quantification of fatty acid methyl esters in benzene fraction of Occidental's boiler blowdown water (ppm).

Methyl ester	Concentration (ppm) in original water ^a
C ₆ branched	6.4
C ₆ normal	20
C ₇ normal	29.5
C ₈ normal	34.6
C ₉ normal	33.1
C ₁₀ normal	27.8
C ₁₁ normal	16.4
C ₁₂ normal	14.8

^a 10m x 0.025mm SP2100 column with C₁₇ methyl ester as internal standard.

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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