IS--4999

DE91 001299

FUNCTIONAL GROUP ANALYSIS IN COAL BY ^{31}P NMR SPECTROSCOPY

Fossil Energy Quarterly Report

January 1, 1989 - March 31, 1989

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Date Transmitted: May 1989

Prepared for: Pittsburgh Energy Technology Center
Pittsburgh, Pennsylvania

*Operated for the U. S. Department of Energy by Iowa State University under Contract No. W-7405-ENG-82.

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ABSTRACT

The purpose of this research is to determine the labile-hydrogen functional group composition of coal and coal-derived materials by the nmr spectroscopy of their derivatives made with reagents containing the nmr-active nuclei ^{31}P, ^{119}Sn, or ^{205}Tl.

This project is funded for one FTE and a qualified replacement for our postdoctoral research associate, Dr. Lensink, who left in December, could not be found in time. Since Dr. Reinartz arrived on the scene March 11, 1989, he has begun syntheses of some of the reagents. Progress of his work will be summarized in next quarter's report.

DEVELOPMENT OF INSTRUMENTAL TECHNIQUES FOR SURFACE ANALYSIS: FUNCTIONAL GROUP ANALYSIS IN COAL BY ^{31}P NMR SPECTROSCOPY

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OBJECTIVE

The purpose of this research is to determine the labile-hydrogen functional group composition of coal and coal-derived materials by the nmr spectroscopy of their derivatives made with reagents containing the nmr-active nuclei ^{31}P, ^{119}Sn, or ^{205}Tl.

INTRODUCTION

Oxygen, sulfur and nitrogen play a very important role in coal processing, consequently rendering it necessary to acquire a knowledge of the forms in which these heteroatoms appear in coal (1). The oxidation of coal during weathering can have a significant deleterious economic impact on coal recovery by froth flotation and oil agglomeration (2) and also on its caloric content in its utilization as a fuel (3). The phenolic and carboxylic acid groups created in weathering appear to have an adverse effect on froth flotation owing to the influence these groups have on the wettability and electrokinetic properties of coal (4).

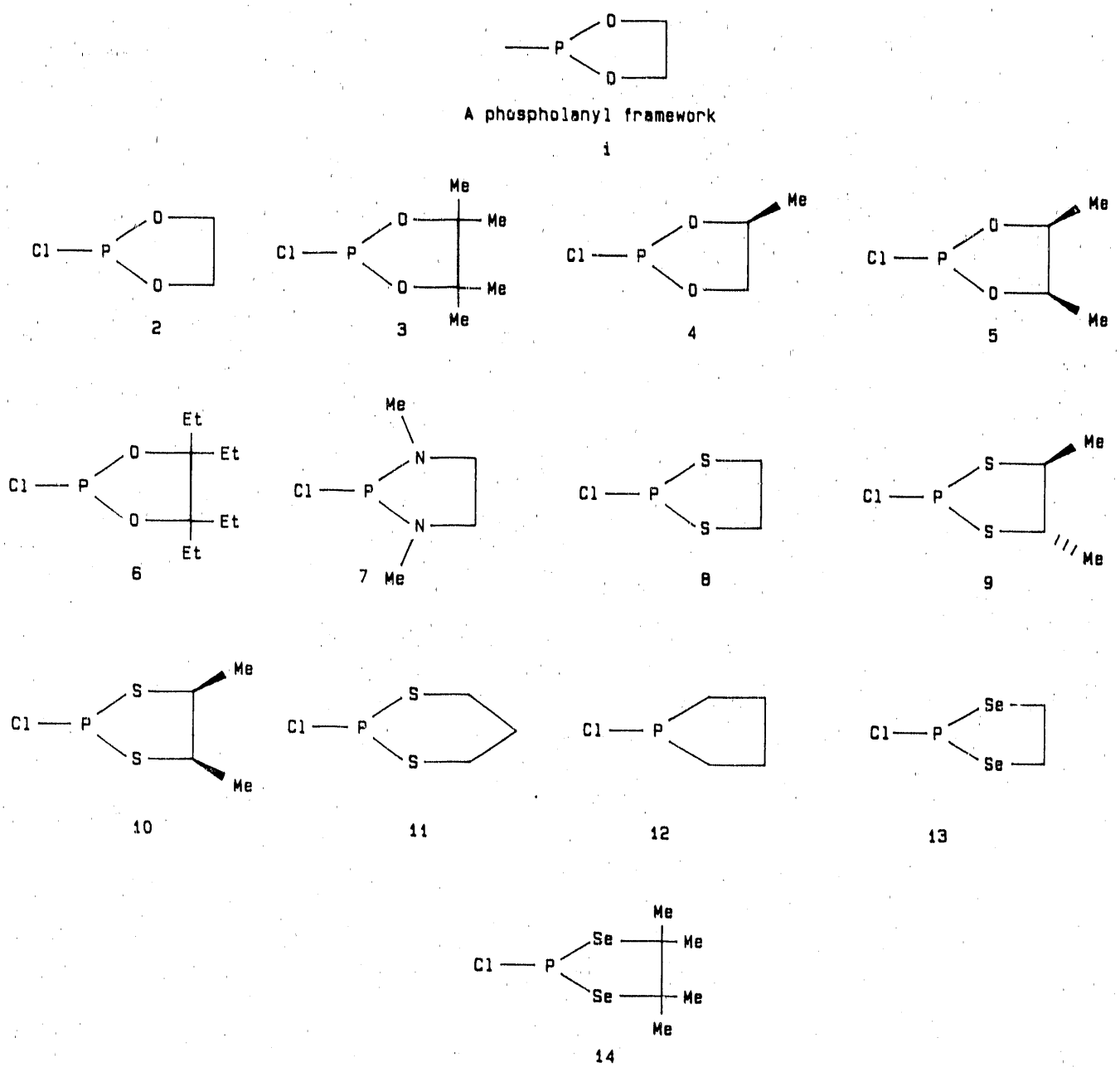
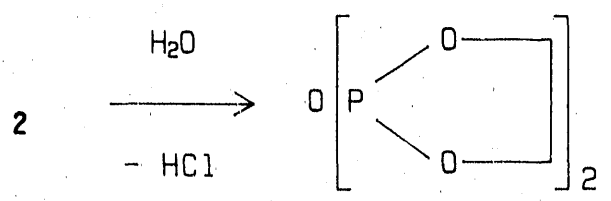
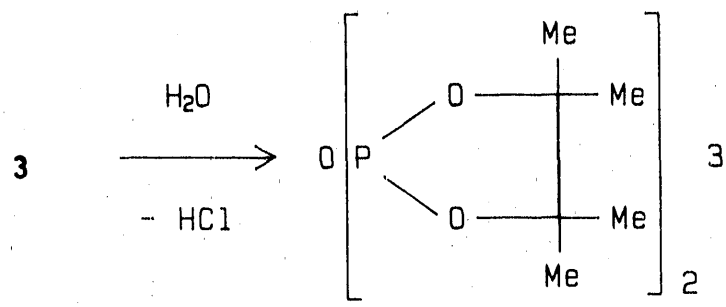


Figure 1. Structures of Phosphorus-Containing Reagents.

During 1988, we serendipitously discovered that reagents such as **2** and **3** react with water to give products whose tentative structures are shown below with their characteristic ^{31}P nmr peaks. We need to verify these structures unambiguously in order to get the analysis for moisture in coals and coal surfaces (an unanticipated bonus) on a sure footing.



31-P = 121.85 (1)



31-P = 132.82 (2)

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2. Z. Sadowski, R. Venkatadri, J. M. Druding, R. Markuszewski, and T. D. Wheelock, Coal Preparation **1988**, 6, 17).

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