



DE85012430

**NTIS**

One Source. One Search. One Solution.

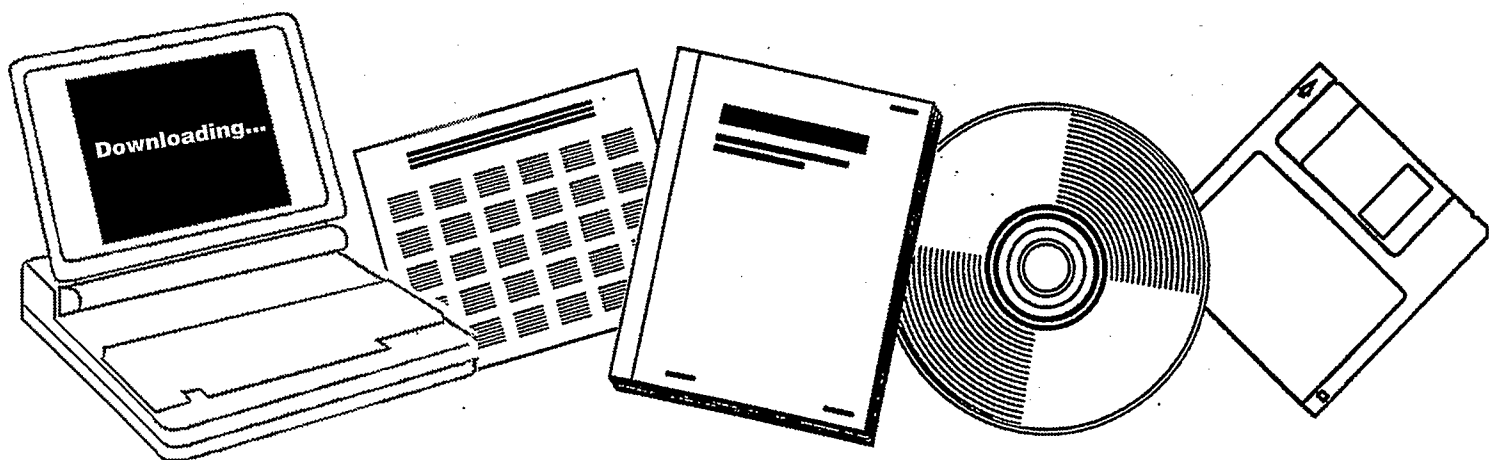
---

---

# FTIR STUDIES OF HYDROCARBON SYNTHESIS ON PD/ZSM5 CATALYSTS. QUARTERLY PROGRESS REPORT

NOTRE DAME UNIV., IN. DEPT. OF CHEMICAL  
ENGINEERING

15 MAY 1985



U.S. Department of Commerce  
**National Technical Information Service**

---

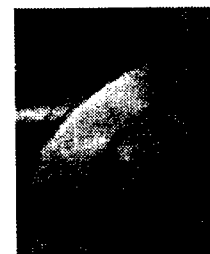
**One Source. One Search. One Solution.**

# NTIS



## **Providing Permanent, Easy Access to U.S. Government Information**

National Technical Information Service is the nation's largest repository and disseminator of government-initiated scientific, technical, engineering, and related business information. The NTIS collection includes almost 3,000,000 information products in a variety of formats: electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.



### **Search the NTIS Database from 1990 forward**

NTIS has upgraded its bibliographic database system and has made all entries since 1990 searchable on [www.ntis.gov](http://www.ntis.gov). You now have access to information on more than 600,000 government research information products from this web site.

### **Link to Full Text Documents at Government Web Sites**

Because many Government agencies have their most recent reports available on their own web site, we have added links directly to these reports. When available, you will see a link on the right side of the bibliographic screen.

### **Download Publications (1997 - Present)**

NTIS can now provide the full text of reports as downloadable PDF files. This means that when an agency stops maintaining a report on the web, NTIS will offer a downloadable version. There is a nominal fee for each download for most publications.

For more information visit our website:

**[www.ntis.gov](http://www.ntis.gov)**



U.S. DEPARTMENT OF COMMERCE  
Technology Administration  
National Technical Information Service  
Springfield, VA 22161

DOE/PC/70788--T1

DOE/PC/70788--T1

DE85 012430

DEPARTMENT OF ENERGY

Quarterly Progress Report

May 15, 1985

Project 84PC70788-2

FTIR Studies of Hydrocarbon Synthesis  
on Pd/ZSM5 Catalysts

directed by

Eduardo E. Wolf  
Professor

Department of Chemical Engineering  
University of Notre Dame

FG 22 - 84 PC 70788

950 7165

**DISCLAIMER**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

### Brief Summary of progress

During the past quarter two tasks were accomplished:

- i) Obtaining reaction rate data in both the Pd/ZSM5 and Pd/SiO<sub>2</sub> catalysts,
- ii) Obtaining infrared spectrum of CO/H<sub>2</sub> mixtures in both of the above catalysts. The results indicate that both catalysts exhibit CO hydrogenation activity but different selectivities. The reaction rate and the selectivities are affected by pressure and temperature. The infrared spectrum of CO on the Pd/ZSM5 catalyst under reaction conditions exhibit several bands which are different than those of adsorbed CO.

### Summary of progress

The two tasks completed during the last quarter were conducted at relatively low pressures, 20 and 75 psi, and the kinetics and IR studies were conducted separately. Leaks had prevented to collect the data in the IR-cell reactor as originally intended, consequently, it was decided to obtain preliminary reaction rate data in the reactor with blank seals instead of the IR transparent windows. These data were obtained on a Pd/ZSM5 and Pd/SiO<sub>2</sub> catalysts in order to ascertain the role of the support. The data summarized in figs. 1-2 show reaction rates and selectivities obtained at five different temperatures and at 20 (atmospheric) and 75 psi total pressure. It can be seen that the rates per unit gram of catalysts are similar in both catalysts and increases with pressure and temperature (fig. 1).

The selectivities, shown in fig. 2 indicate that the ZSM5 support indeed affects the reaction pathway by producing a different product distribution than the SiO<sub>2</sub> supported Pd. The zeolite support leads to heavier hydrocarbons than the silica support at 250-300°C, but the cracking acidity of the zeolite predominates at the higher temperature leading to more C<sub>1</sub> (fig. 2).

Infrared studies were conducted on the Pd/ZSM5 catalyst under reaction conditions at atmospheric pressure, and at the same temperatures than the

reaction studies. IR spectra were also obtained at 40 psi in a  $N_2$  atmosphere and at various temperatures. Fig. 3 shows the spectrum of a mixture of  $CO/H_2$  under reaction conditions at  $250^\circ C$ . The linear and bridge bonded form of CO adsorbed on Pd can be clearly seen at about  $2071$  and  $1955\text{ cm}^{-1}$ , along with a small peak at  $1593\text{ cm}^{-1}$ . As the temperature increases to the point at which the reaction rate starts increasing with temperature, and production of hydrocarbons other than  $C_1$  is detected, the spectrum changes significantly as shown in fig. 4. The shoulder, which is barely seen in the bridge bonded band in fig. 3, develops as a separate band centered at  $1859\text{ cm}^{-1}$ . Furthermore, the band at  $1593\text{ cm}^{-1}$  fully develops centered at  $1578\text{ cm}^{-1}$  along with a similar band at  $1477\text{ cm}^{-1}$ .

The band adjacent to the bridge bonded peak increases with temperature but decreases again as the temperature decreases. However, the low frequency bands once formed, are not strongly affected by temperature or the reaction environment.

The IR results obtained at 40 psi under a  $CO/N_2$  atmosphere show bands located at similar frequencies as those obtained at 1 atm. and under  $CO/H_2$ , although in this case, the gas phase CO band at  $2183\text{ cm}^{-1}$  predominates (fig. 5). The band at  $1851\text{ cm}^{-1}$  is much less intense and the band at  $1477\text{ cm}^{-1}$  can be barely detected. Since the reaction studies and the IR studies were conducted separately, a clear connection between these two is not yet possible, nonetheless the present data indicates that the ZSM5 catalyst have an hydrogenation function and that adsorbed species other than CO are observable. Work at higher pressures and in the same IR cell reactor is needed to verify if the Pd/ZSM5 catalysts possesses a bifunctional character, which is the main hypothesis of this work, and to identify the nature of the IR bands under reaction conditions.

Figure 1

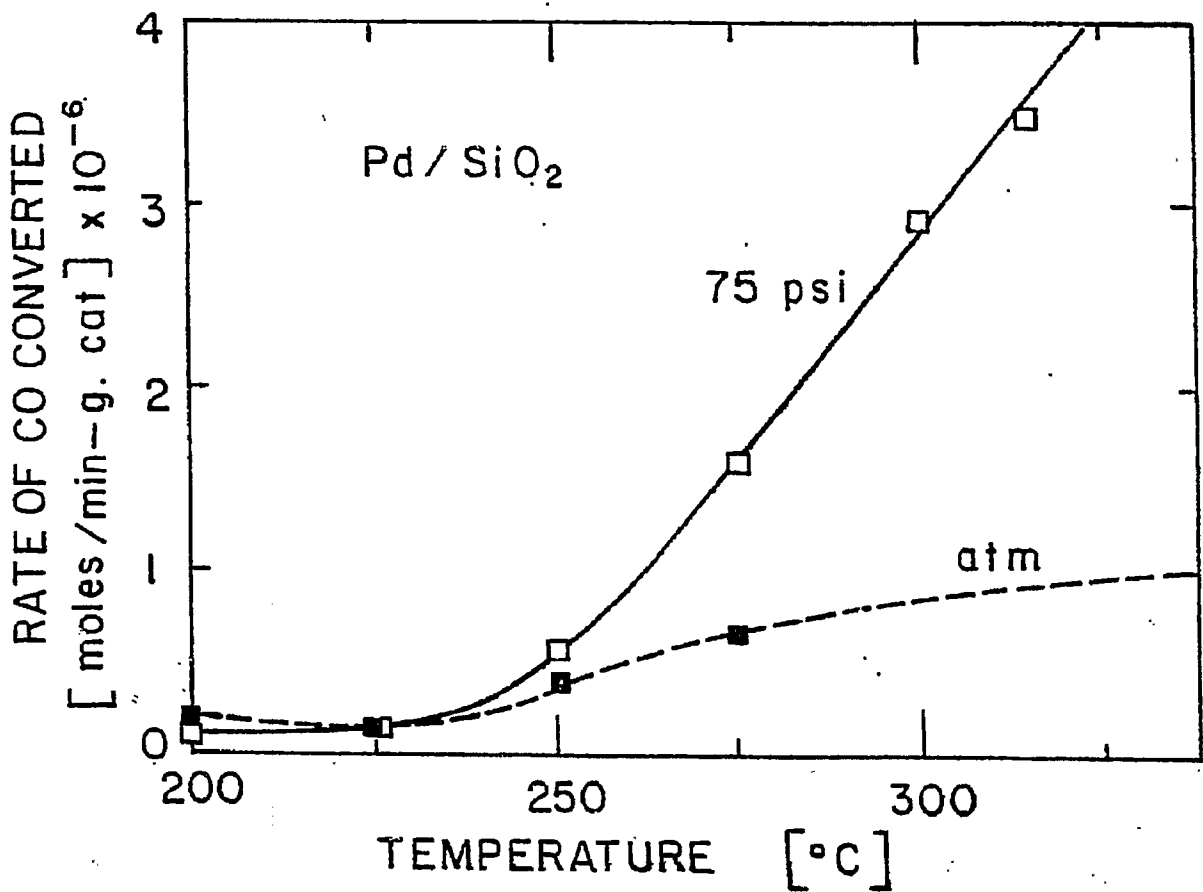
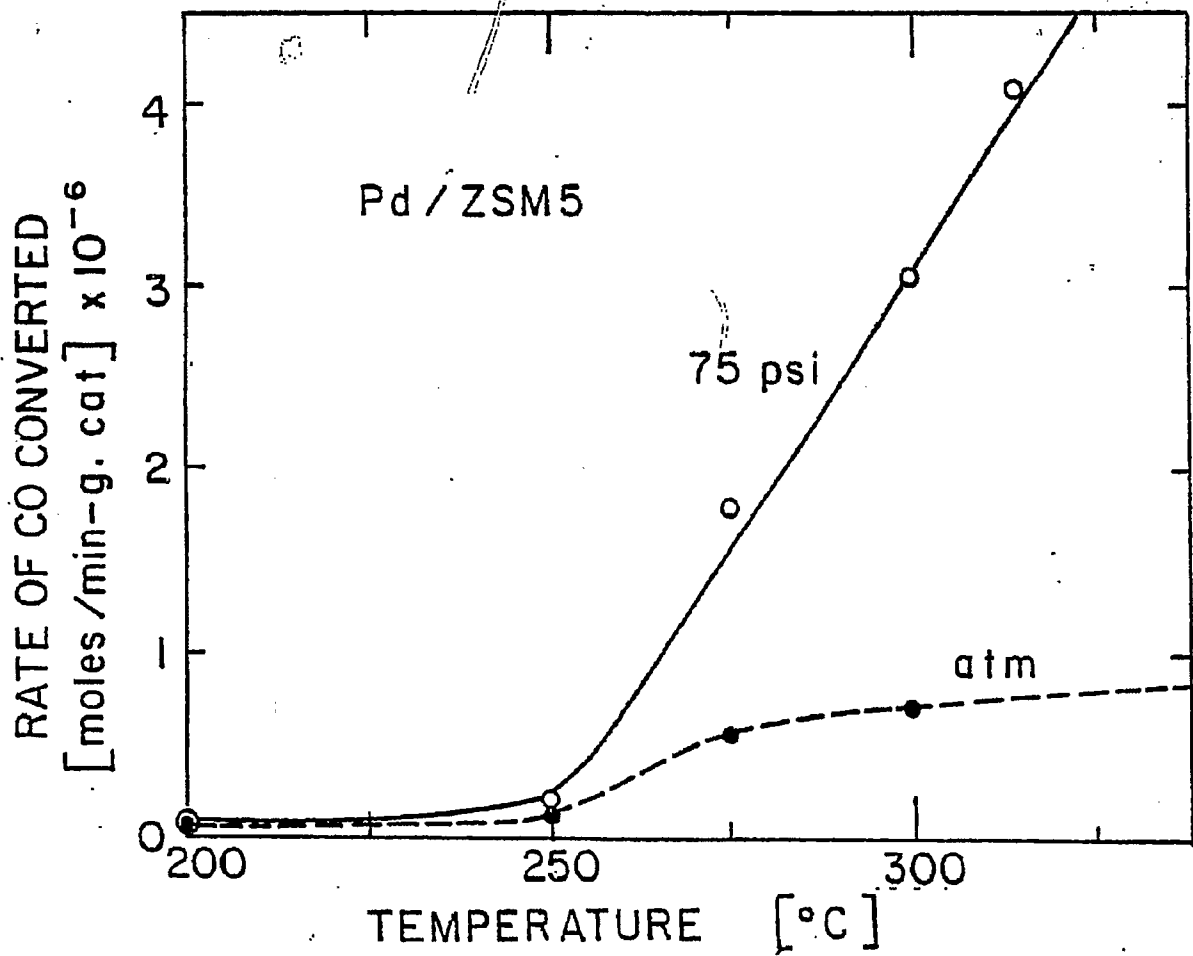
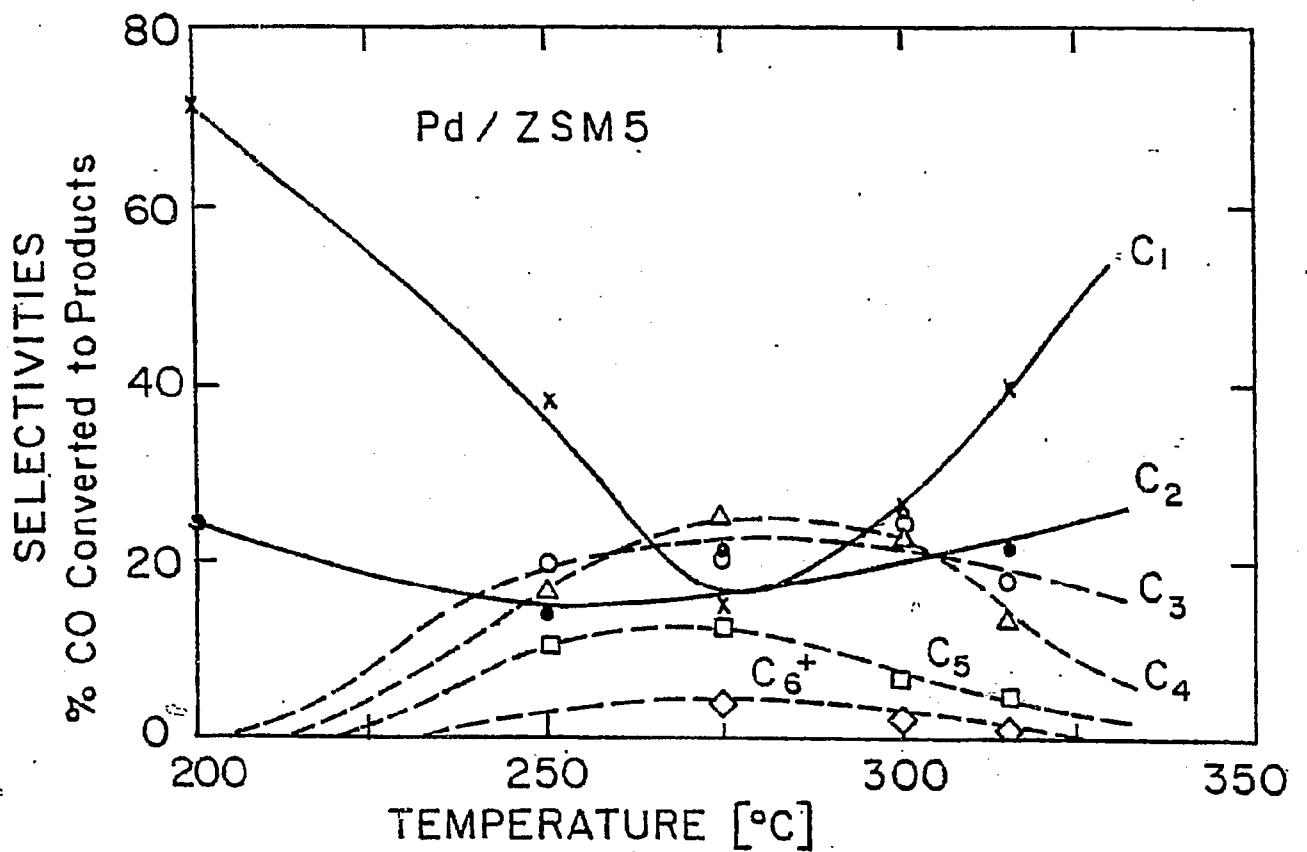
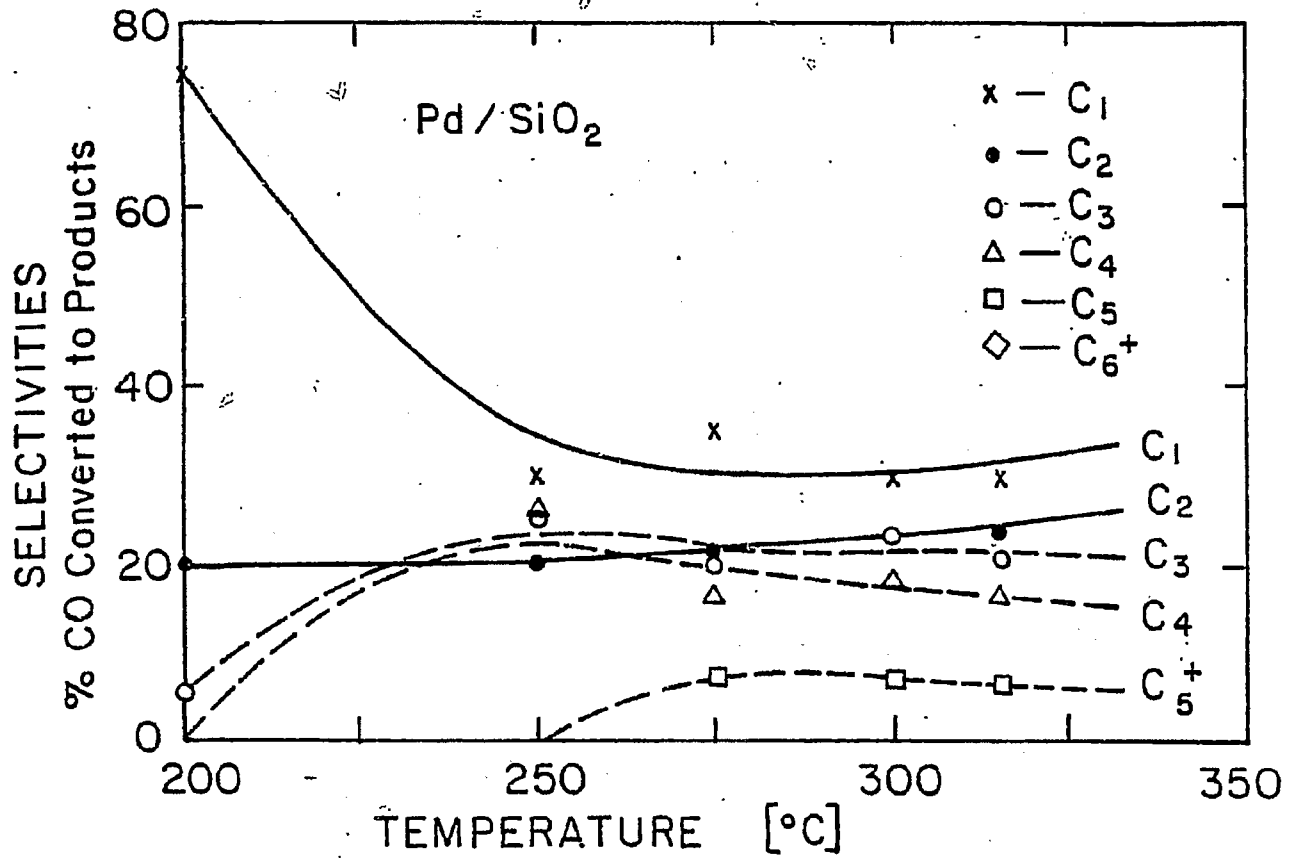
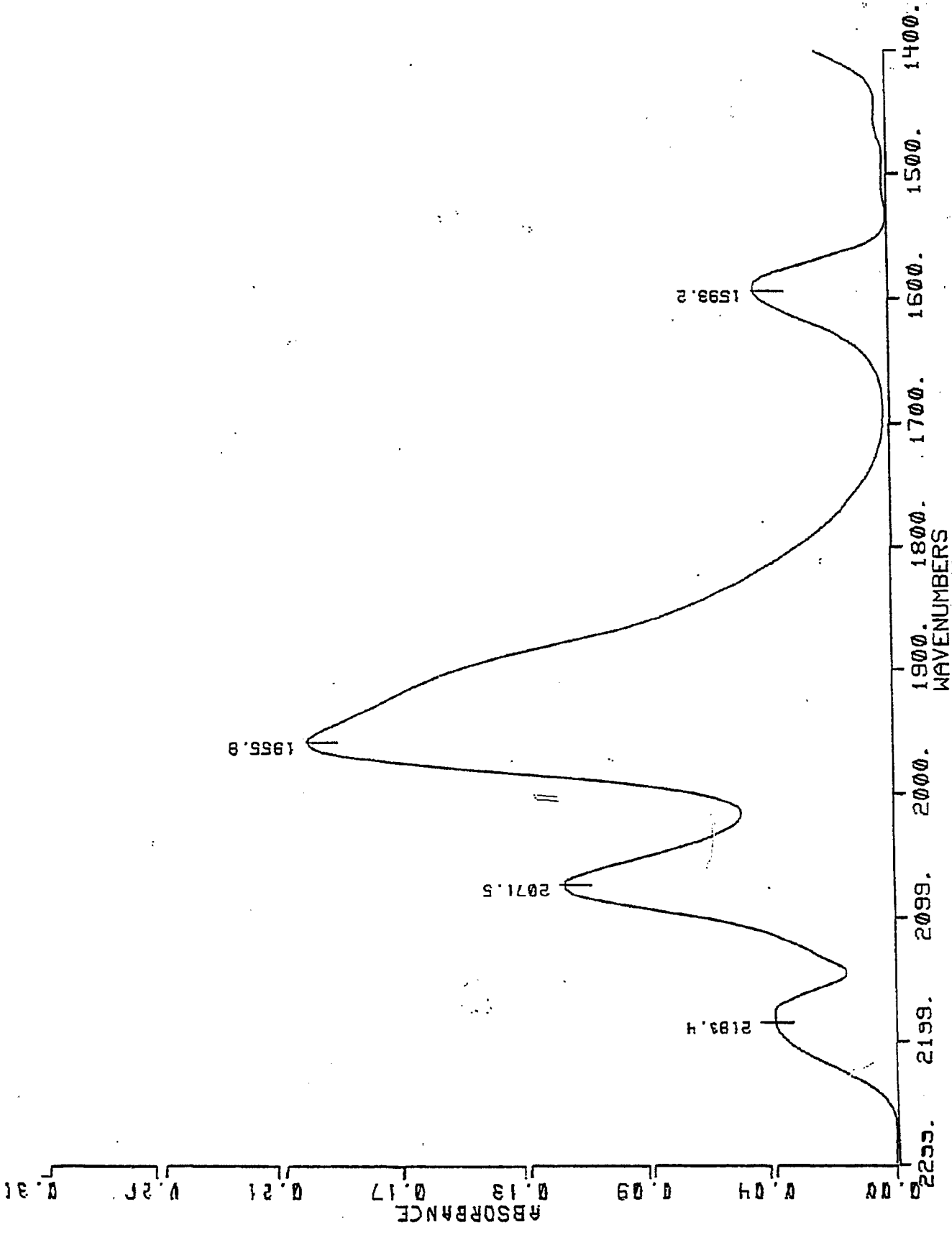


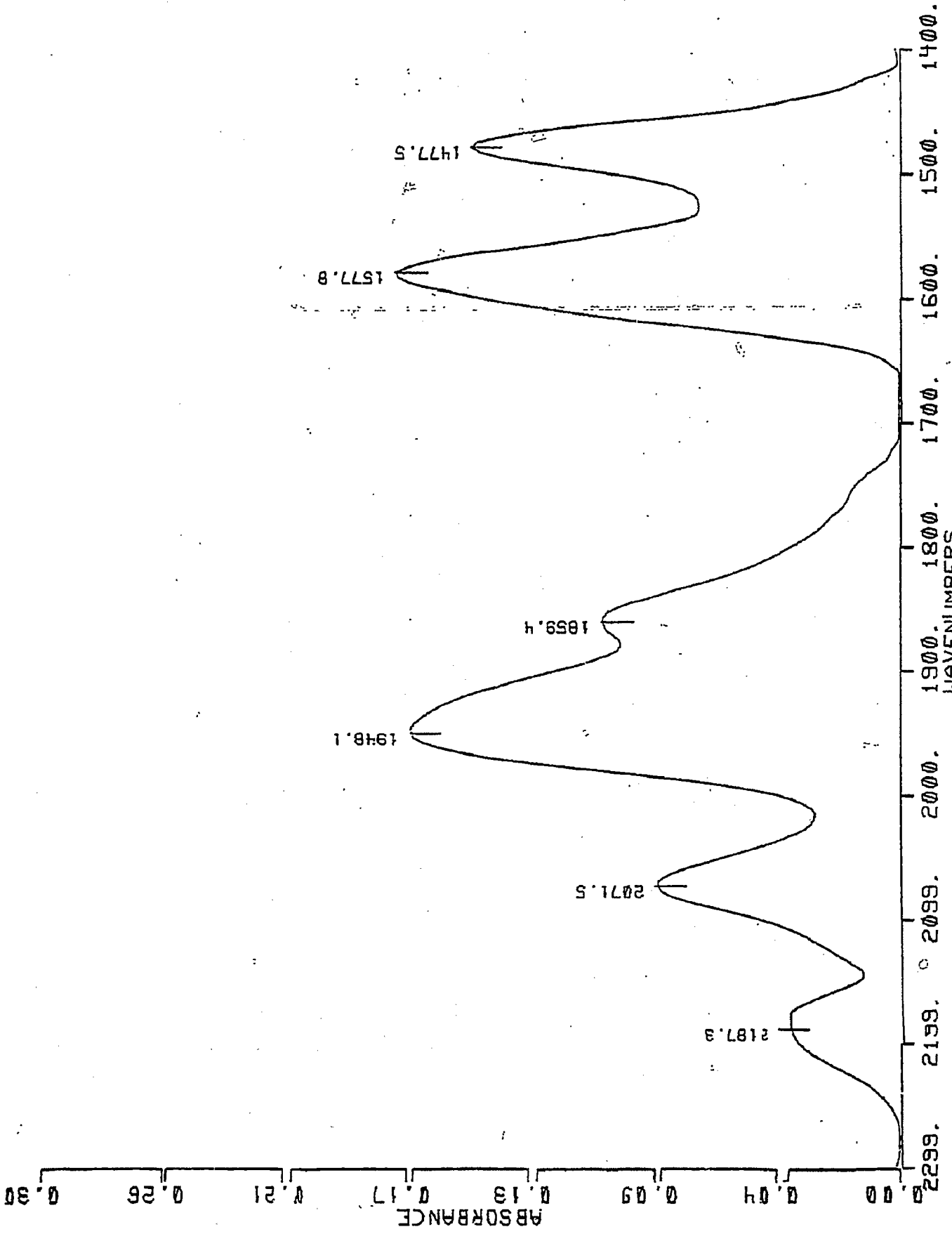
Figure 2



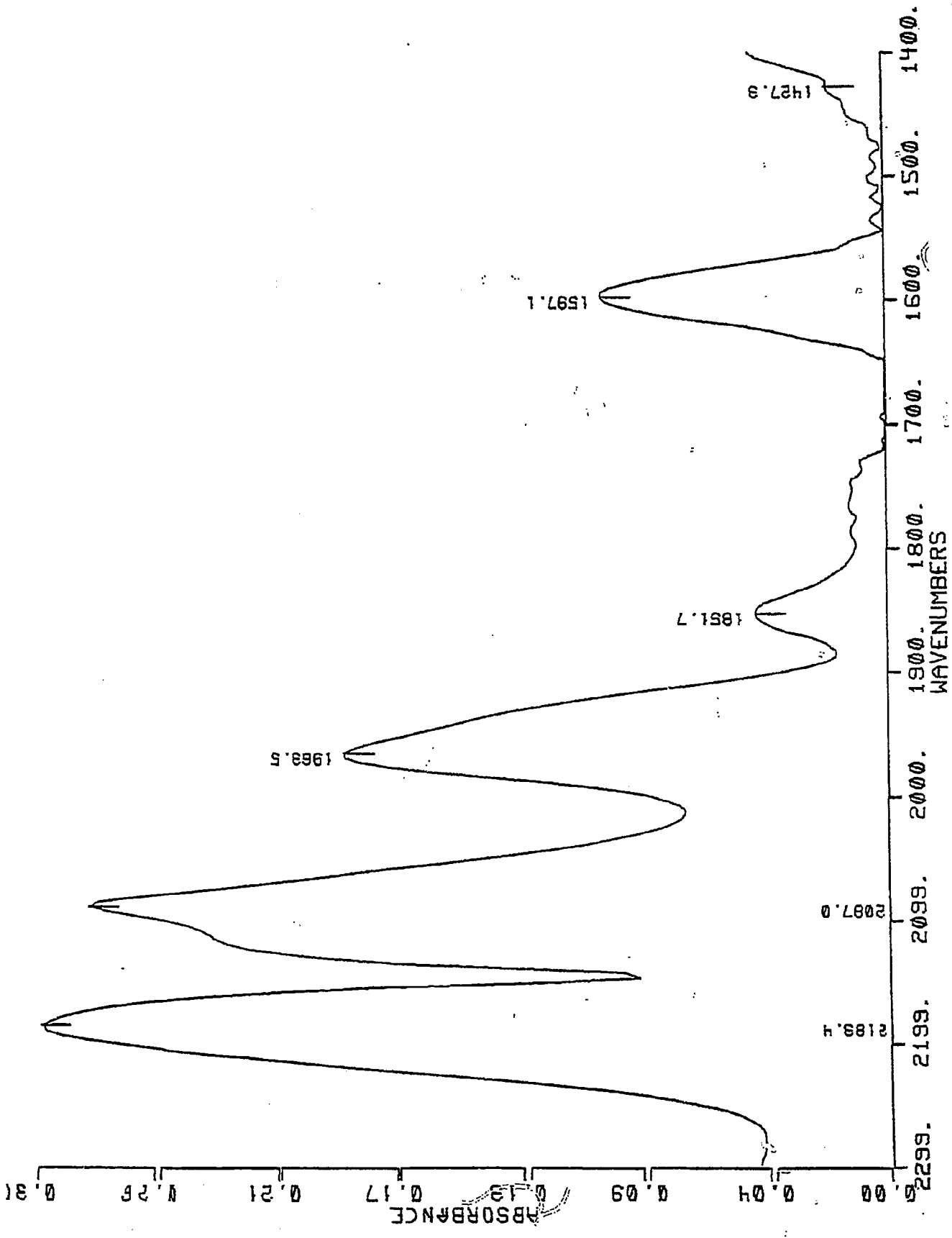


PFA=151  
LEVEL=0.03  
REACTION CONDITIONS T=250 C P=ATM  
Figure 3





PFN=352  
 REACTION CONDITIONS T=275 C P=ATM  
 LEVEL=0.02  
 Figure 4



PFA=15C03 SURFACE UNDER CO/N2 T=270 C P=40 PSI

LEVEL=0.02

Figure 5

## **SATISFACTION GUARANTEED**

**NTIS strives to provide quality products, reliable service, and fast delivery. Please contact us for a replacement within 30 days if the item you receive is defective or if we have made an error in filling your order.**

▲ **E-mail: [info@ntis.gov](mailto:info@ntis.gov)**

▲ **Phone: 1-888-584-8332 or (703)605-6050**

# **Reproduced by NTIS**

National Technical Information Service  
Springfield, VA 22161

***This report was printed specifically for your order from nearly 3 million titles available in our collection.***

For economy and efficiency, NTIS does not maintain stock of its vast collection of technical reports. Rather, most documents are custom reproduced for each order. Documents that are not in electronic format are reproduced from master archival copies and are the best possible reproductions available.

Occasionally, older master materials may reproduce portions of documents that are not fully legible. If you have questions concerning this document or any order you have placed with NTIS, please call our Customer Service Department at (703) 605-6050.

## **About NTIS**

NTIS collects scientific, technical, engineering, and related business information – then organizes, maintains, and disseminates that information in a variety of formats – including electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.

The NTIS collection of nearly 3 million titles includes reports describing research conducted or sponsored by federal agencies and their contractors; statistical and business information; U.S. military publications; multimedia training products; computer software and electronic databases developed by federal agencies; and technical reports prepared by research organizations worldwide.

For more information about NTIS, visit our Web site at <http://www.ntis.gov>.

# **NTIS**

**Ensuring Permanent, Easy Access to  
U.S. Government Information Assets**



U.S. DEPARTMENT OF COMMERCE  
Technology Administration  
National Technical Information Service  
Springfield, VA 22161 (703) 605-6000

---