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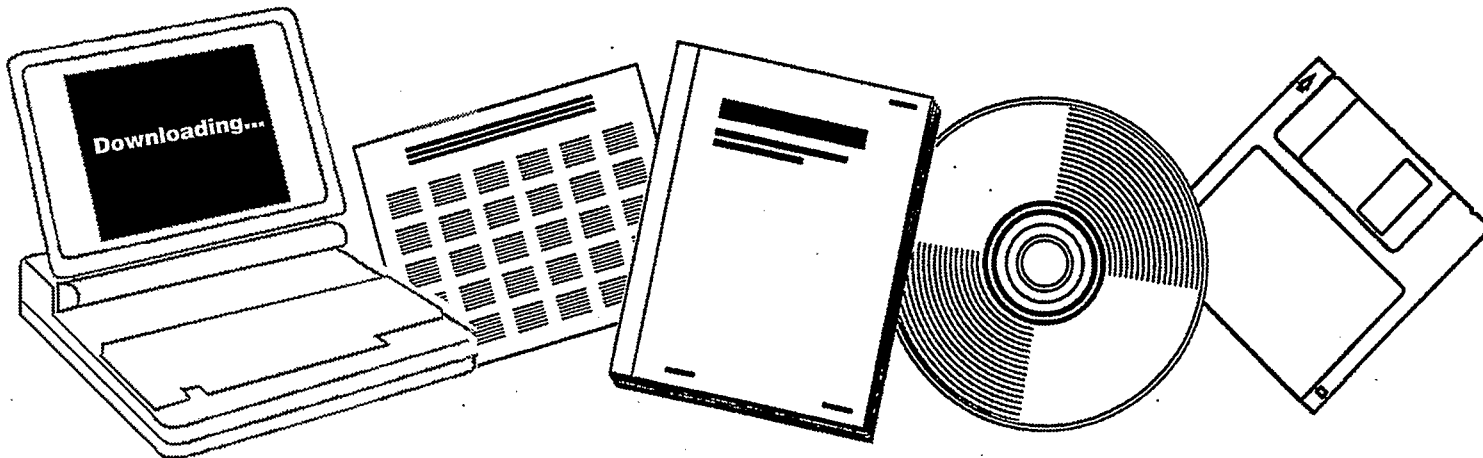
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**FTIR STUDIES OF HYDROCARBON SYNTHESIS ON
PD/ZSM5 CATALYSTS. QUARTERLY PROGRESS
REPORT, AUGUST 15, 1985**

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

15 AUG 1985



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DEPARTMENT OF ENERGY

Quarterly Progress Report

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Project 84PC70788-2

FTIR Studies of Hydrocarbon Synthesis
on Pd/ZSM5 Catalysts

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Brief summary of progress

During the last quarter several objectives were attained:

- 1) Pd/ZSM5 catalysts are capable of methanol and hydrocarbon synthesis
- 2) The temperature and pressure dependence of the reaction rates were established. The reaction rate increases with temperature and pressure, and is independent of residence time.
- 3) Methanol yield reaches a maximum as pressure increases, and it decreases as temperature increases.
- 4) Ir spectra are dominated by the linear and bridge bonded forms of CO, as well as by bands at 1550- 1400 cm^{-1} .

Summary of progress

Results demonstrating the first two objectives indicated above are displayed in figs. 1-3 in terms of reaction rates versus the corresponding operating variable. Figures 4-6 show the effect of the same variables in the product distribution. Methanol production follows a trend characteristic of a reaction intermediate, which suggest that the catalyst is apparently operating via a bifunctional mechanism.

A typical IR spectrum at low pressure (50 psi), shown in fig. 7, indicate that the prevailing bands are those corresponding to gas phase CO, a band at 1932 due to linearly adsorbed CO, and non identified bands at 1712, 1523, 1442, and 1404 cm^{-1} . As pressure increases, the gas phase CO bands become very large and overtake the linearly adsorbed CO band. The effect of pressure and temperature in the low frequency bands are shown in figs 8-9. While pressure does not affect significantly these bands, temperature changes their relative proportions.

Current work is addressing at the chemical identification of the observed bands, as well as their correlation with the activity and selectivity patterns to establish the reaction pathway.

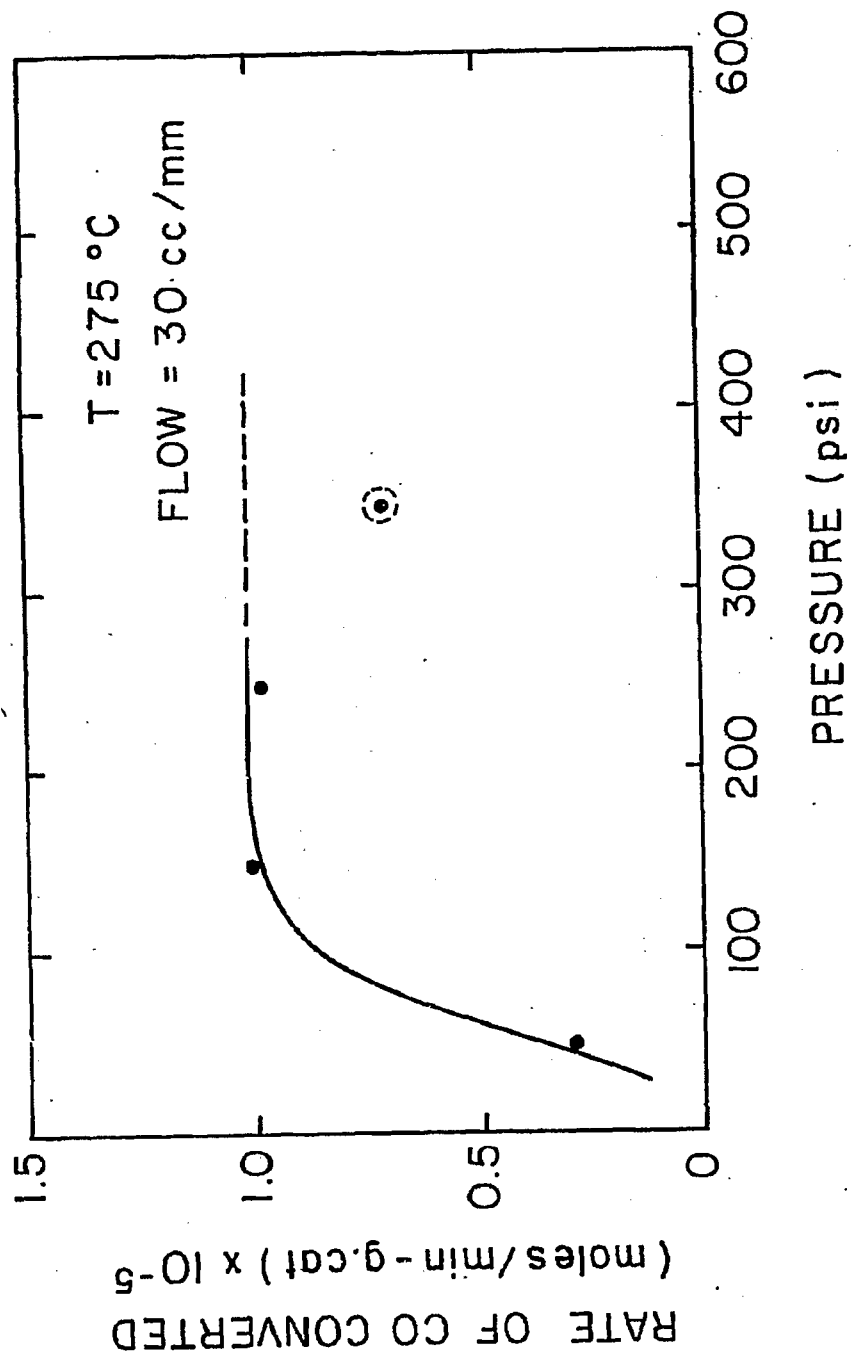


Figure 1

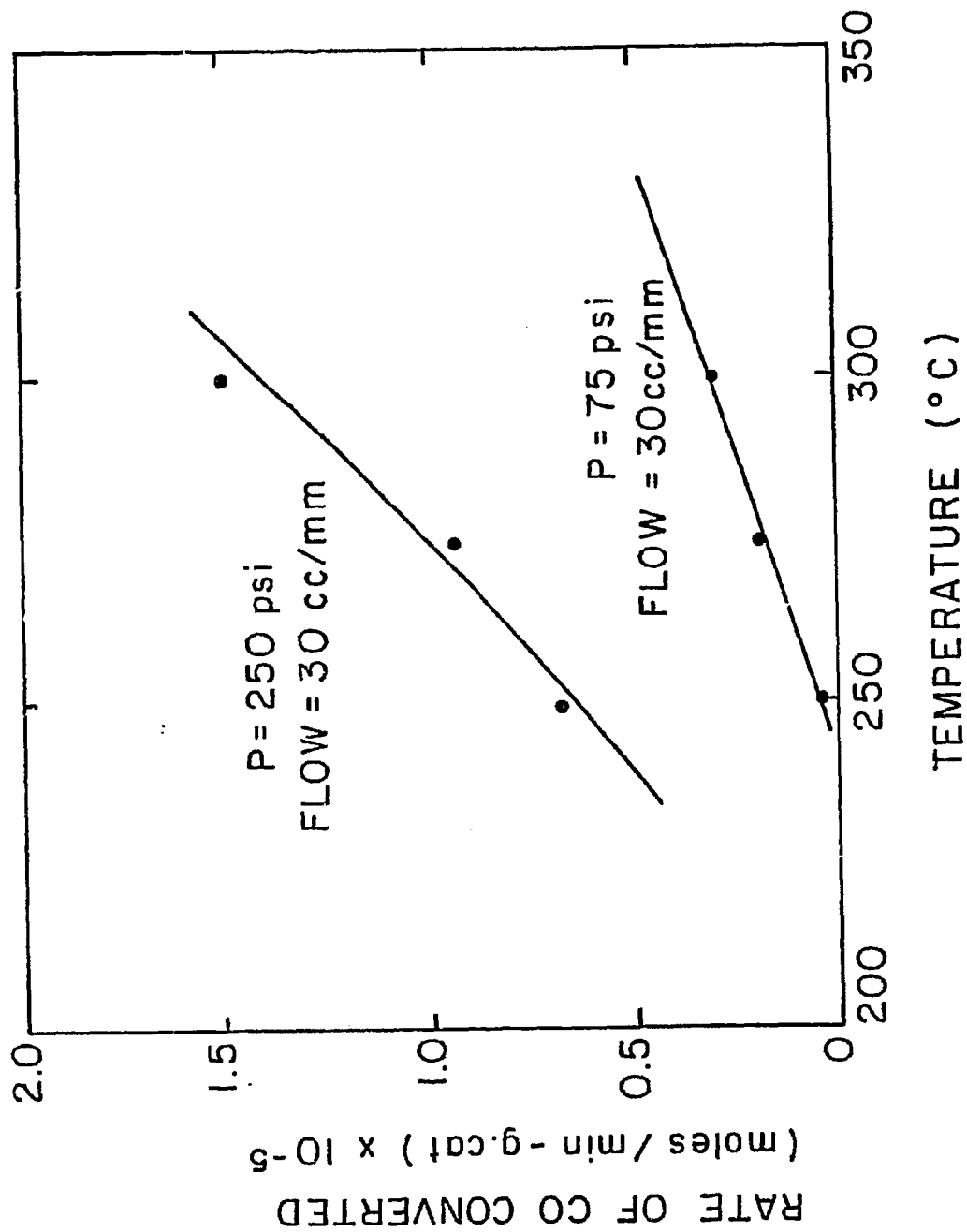


Figure 2

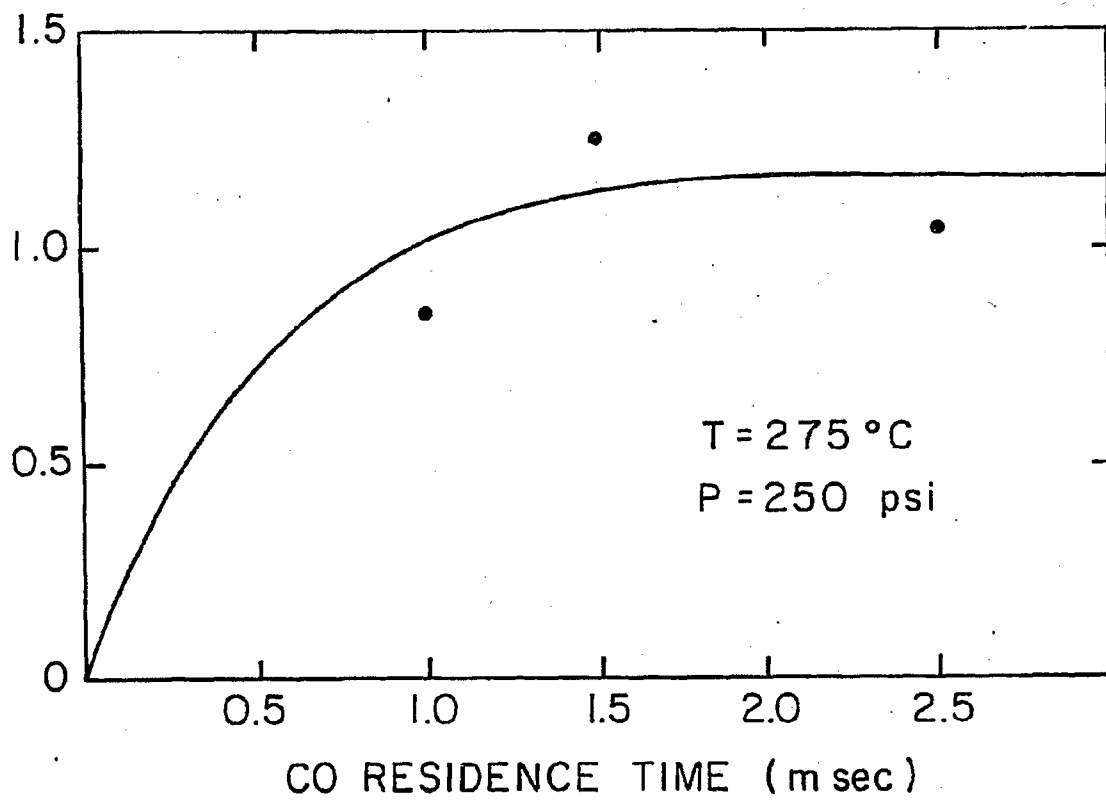


Figure 3

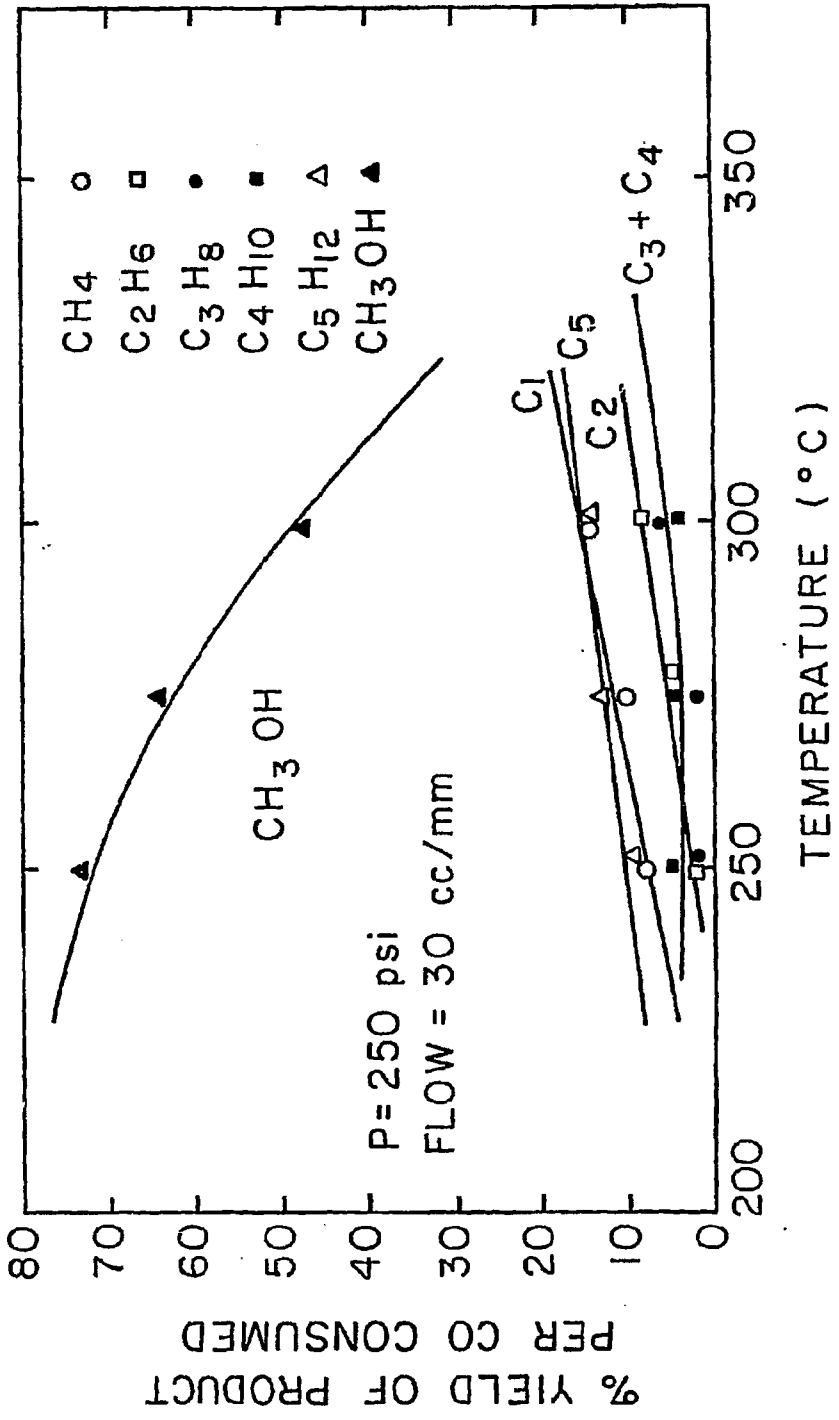


Figure 4

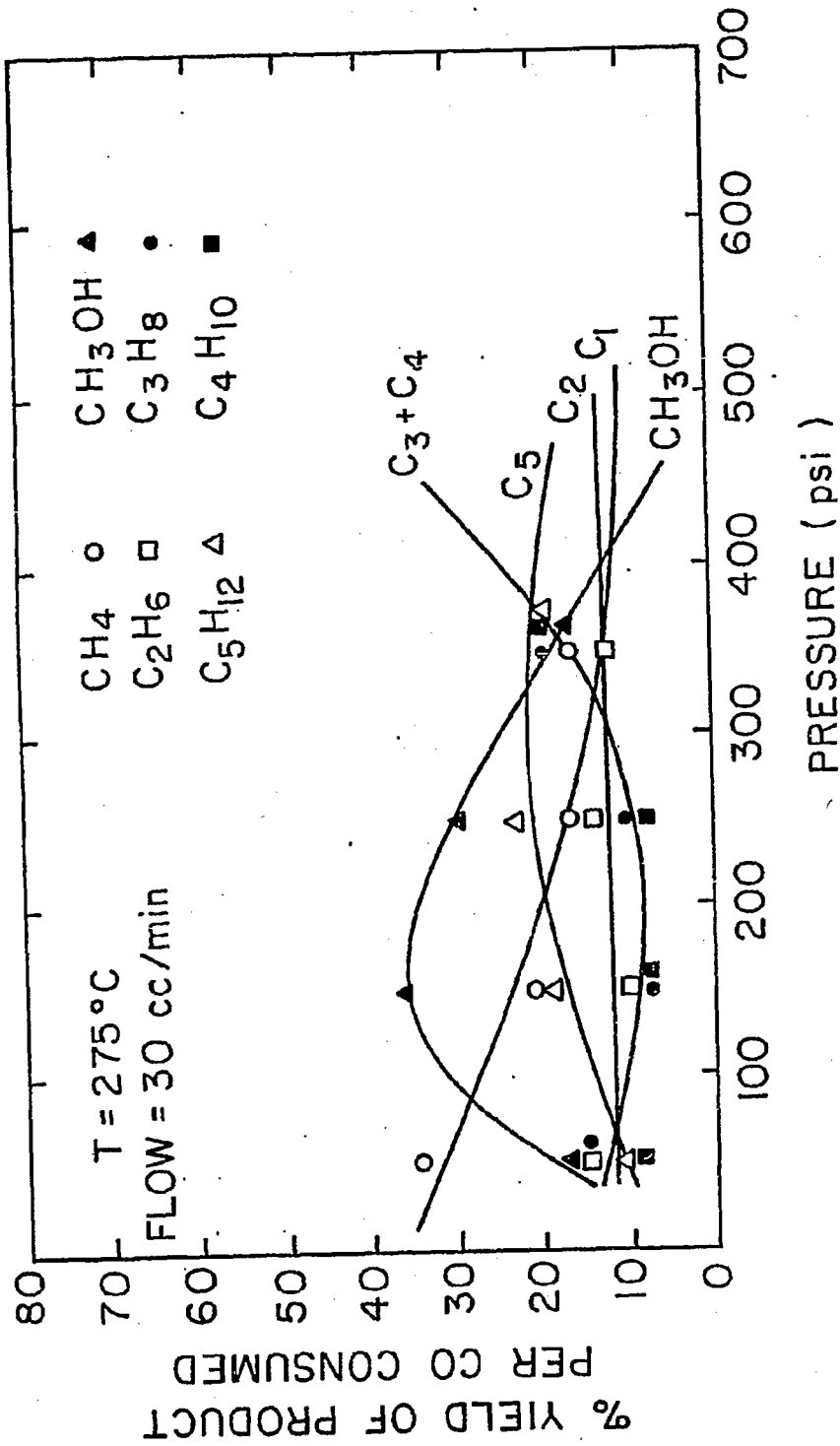


Figure 5

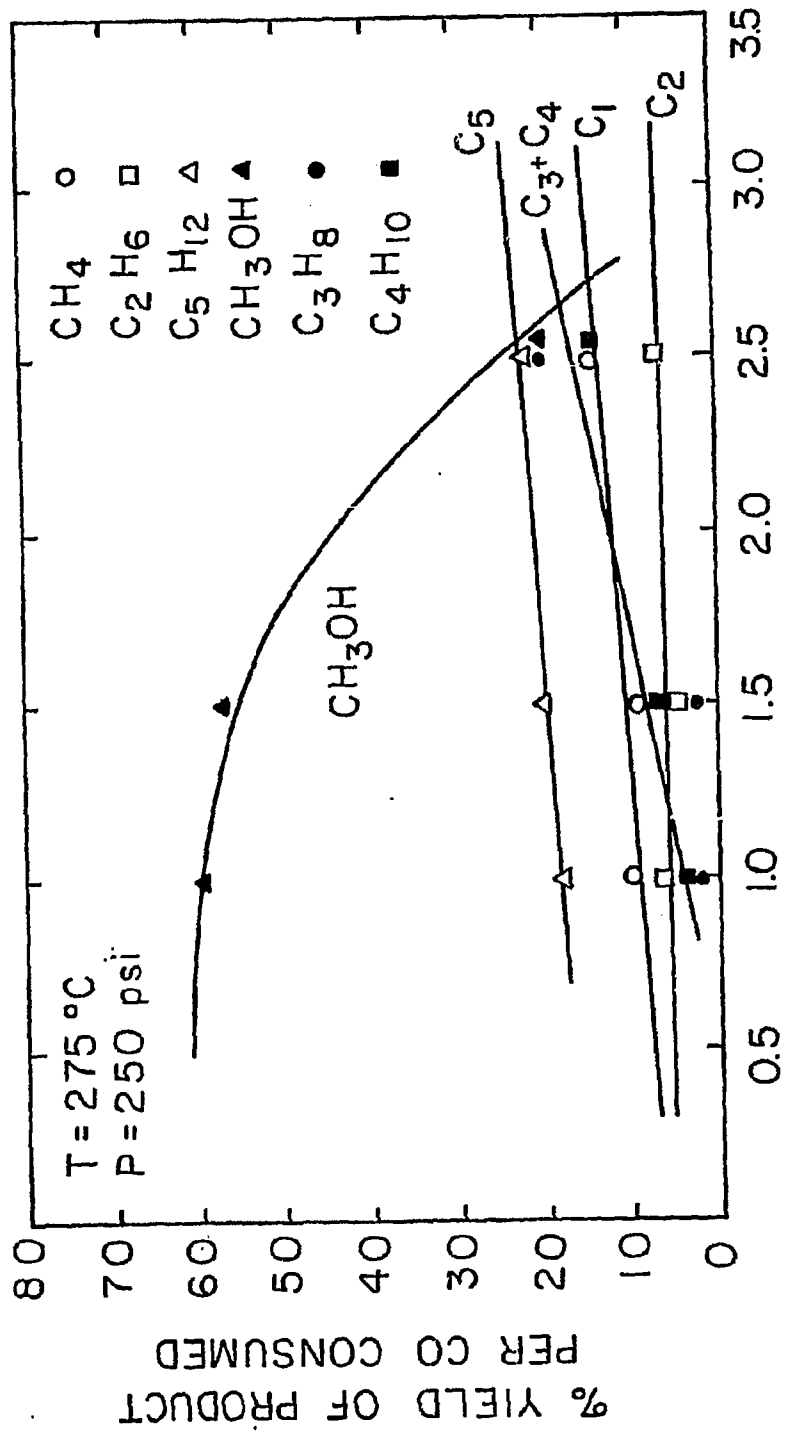
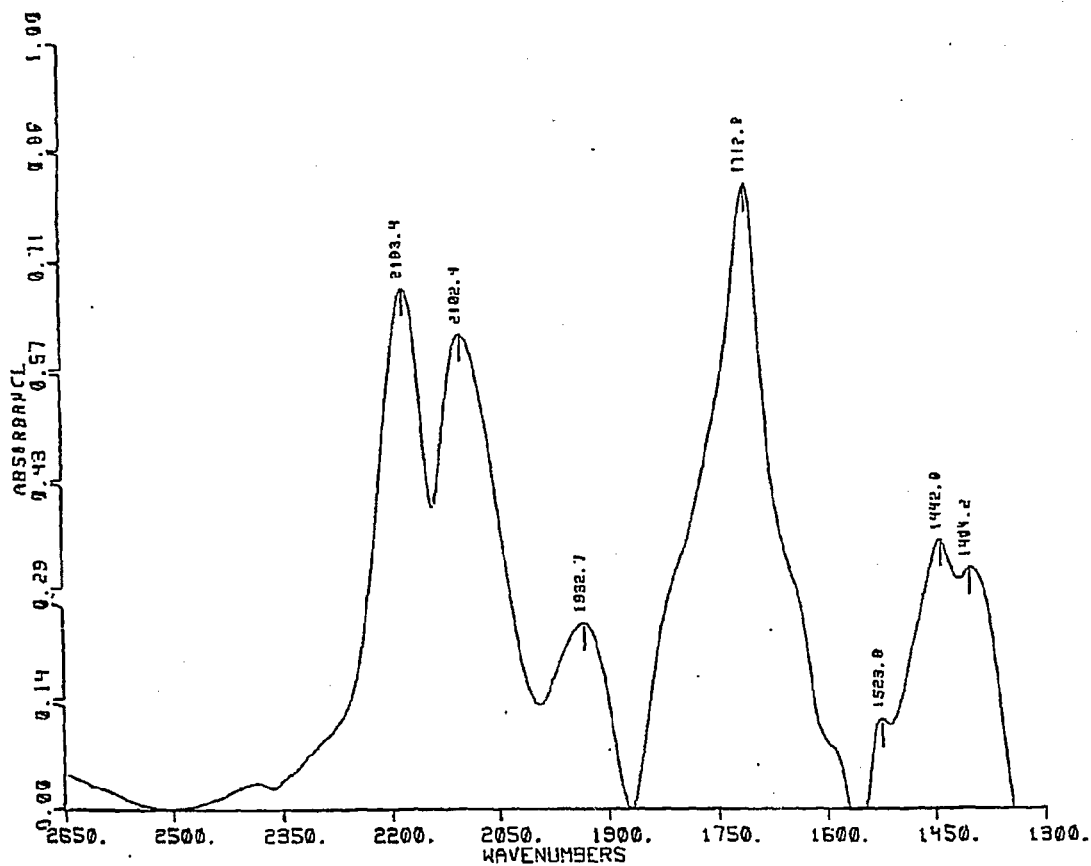


Figure 6

Figure 7



IR SPECTRA OF CATALYST DURING RXN 275 C 50 PSI

IR SPECTRA OF CATALYST WAFER UNDER REACTION CONDITIONS

Figure 8

T=275 C
FLOW=30 ML/MIN

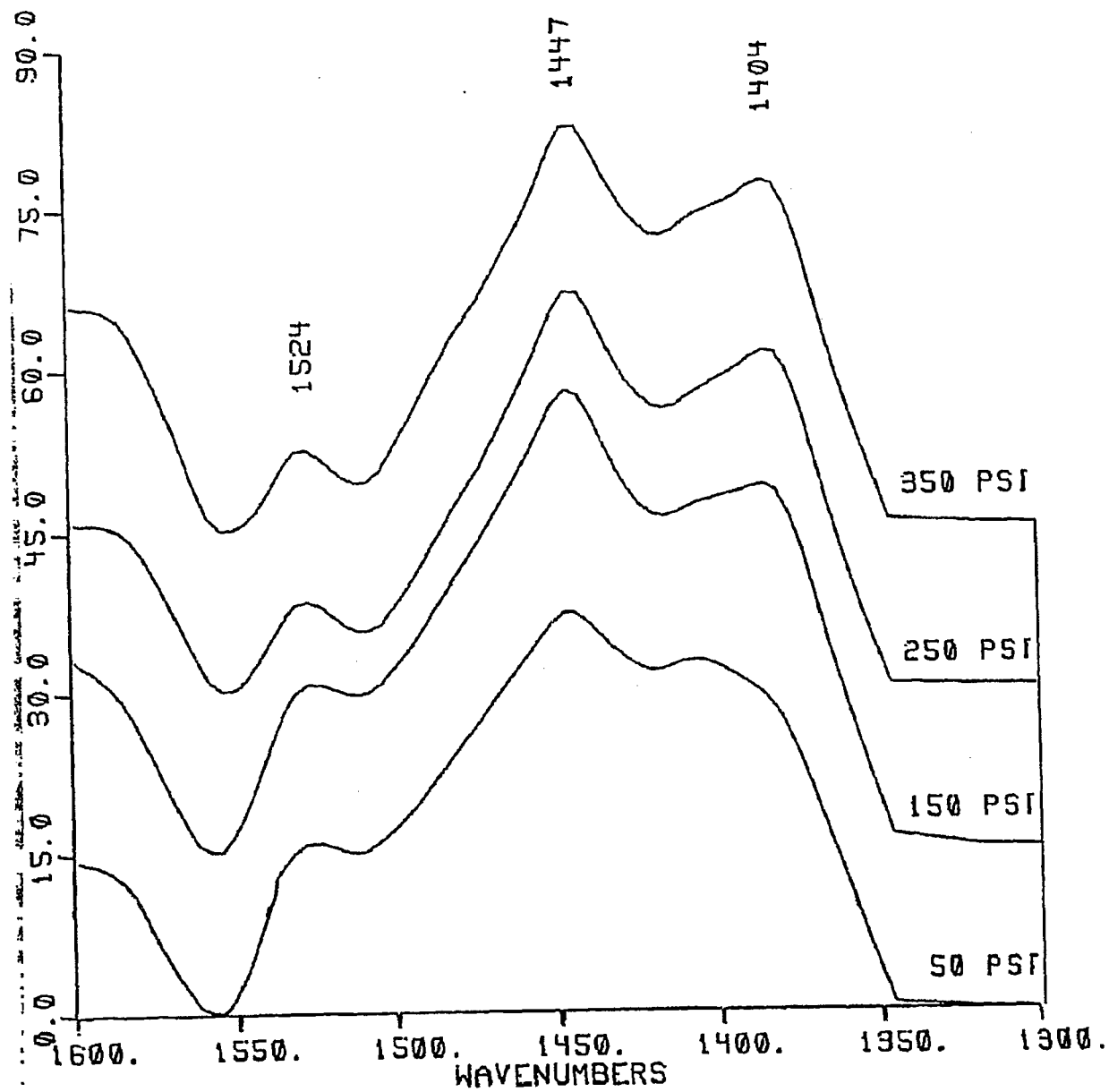
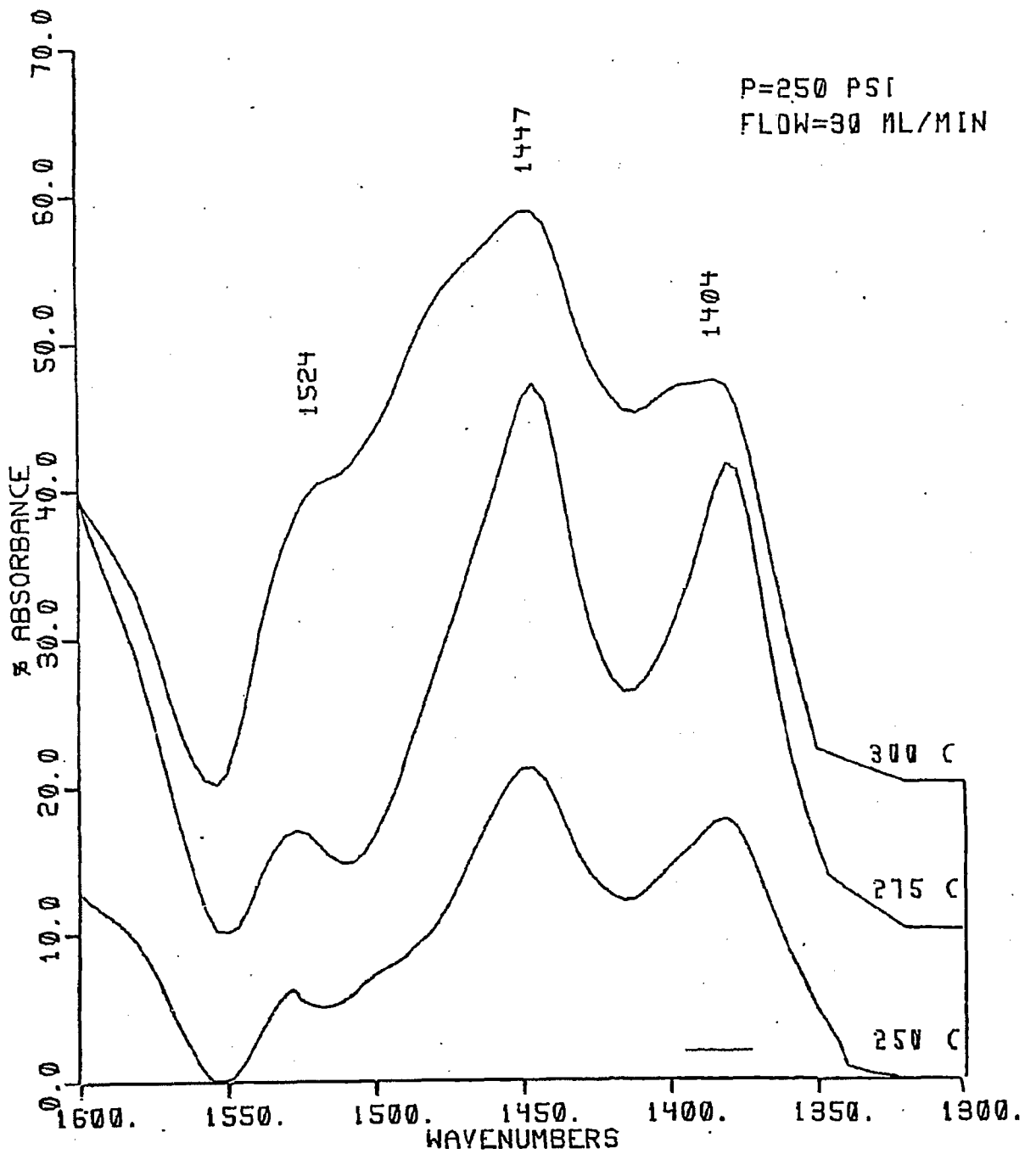


Figure 9
IR SPECTRA OF CATALYST WAFER
UNDER REACTION CONDITIONS



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