

Figure 7. X-Ray diffraction patterns for unsupported Co (a), CoB-109G (b), and Co/Na (c, d) catalysts.

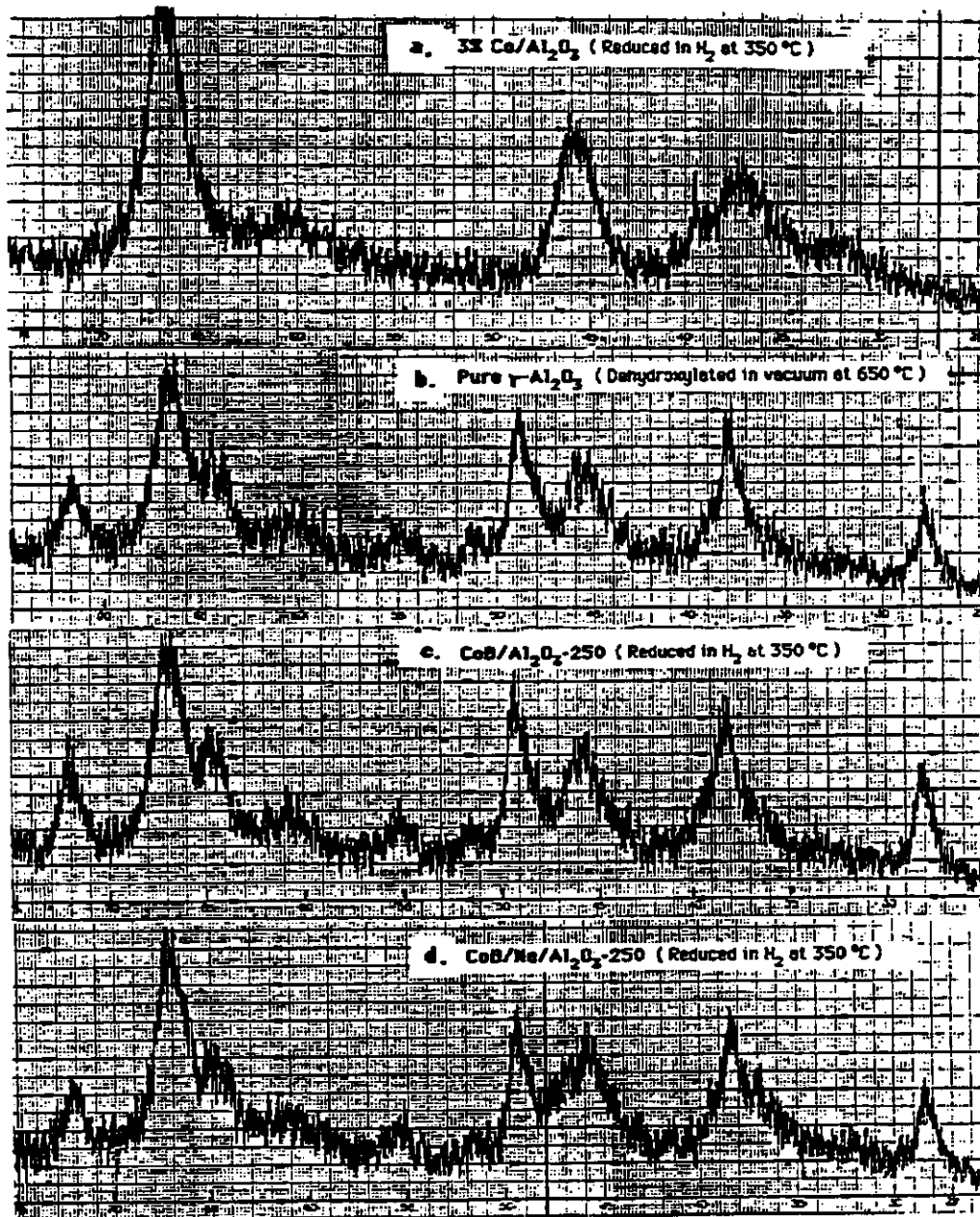


Figure 8. X-Ray diffraction patterns for 3% Co/ Al_2O_3 catalysts (a), pure γ - Al_2O_3 (b), CoB/ Al_2O_3 (c), and CoB/Na/ Al_2O_3 -250 (d).

contained no clear evidence of either cobalt metal or the cobalt boride phases in alumina-supported Co, CoB or CoB/Na catalysts since it is difficult to use x-ray diffraction for phase analysis of such fine particles in the presence of a large amount of alumina (cobalt metal loading 3-3.8 wt%). The x-ray pattern for pure γ -alumina dehydroxylated at 650 °C showed not only the main peaks for γ -alumina itself but also other peaks appearing at $2\theta = 28.4^\circ$, 49.2° , 51.6° , 55.1° , 65.0° , and 71.8° which are unidentifiable with any other possible form of alumina listed in the ASTM x-ray diffraction index cards. These unidentifiable peaks probably resulted from the structural change in the alumina during dehydroxylation at 650 °C.

During the fourth year of the contract, TPD studies of CO from cobalt borides were conducted to determine the effects of boron on the adsorption binding energies and states. The results illustrated in Figures 9-12 indicate that CO adsorption states are shifted to higher temperatures and binding energies in boron and boron/sodium containing samples relative to cobalt-only samples.

Indeed, previously obtained spectra for CO desorption from unsupported Co contain peak maxima at 100 and 300°C [29], indicative of weakly bound CO. The TPD spectra of CO and CO₂ from unsupported CoB-250 and CoB/Na-250 catalysts after reduction in H₂ at 250 °C are displayed in Figures 9 and 10. CO was adsorbed at 25 °C in all cases. No weakly bound CO species is observed on CoB-250, as the desorption of CO was not detected until after 350 °C. Three strongly bound high temperature peaks are observed at about 400, 450, and 550 °C. Corresponding CO₂ peaks are also observed at about the same temperatures suggesting that CO dissociates allowing the reaction of the surface oxygen with other CO molecules to form CO₂. Figure 10 shows that with Na present in the borided cobalt catalyst, a weakly bound CO species desorbs at about 150 °C CoB/Na-250.

Figure 11 shows the TPD spectra of CO and CO₂ on a 3 wt% Co/Al₂O₃ catalyst reduced in H₂ at 350 °C. After adsorption of CO at 25 °C, two different adsorption states are observed for CO at about 100 °C and 350 °C respectively. The intensity of the moderately bound 350 °C peak is relatively low while a large portion of the adsorbed CO occupies the lower binding energy state and desorbs at temperatures below 180 °C, the typical reaction temperature for CO hydrogenation over cobalt catalyst. Figure 11 also shows that some CO₂ is produced at temperatures above 200 °C indicating that dissociation of CO may occur at elevated temperatures and that some oxygen is released in the form of CO₂.

On the other hand, only high temperature binding states of CO are observed on the CoB/Al₂O₃ catalyst after reduction in H₂ at 250 °C and adsorption of CO at 25 °C. Indeed Figure 12 shows no evidence of the weakly bound CO species during CO TPD from this borided cobalt catalyst while two strongly bound high temperature peaks are observed at about 370 °C and 430 °C which probably correspond to recombination of surface carbon and oxygen since corresponding CO₂ peaks are also detected at about the same position. Thus, comparison of the TPD spectra in Figures 11 and 12 for Co/Al₂O₃ and CoB/Al₂O₃ reveals that addition of boron causes a shift to high temperature binding states of CO. In general, the presence of boron increases the binding energy of CO with cobalt for both unsupported and alumina-supported borided cobalt catalysts.

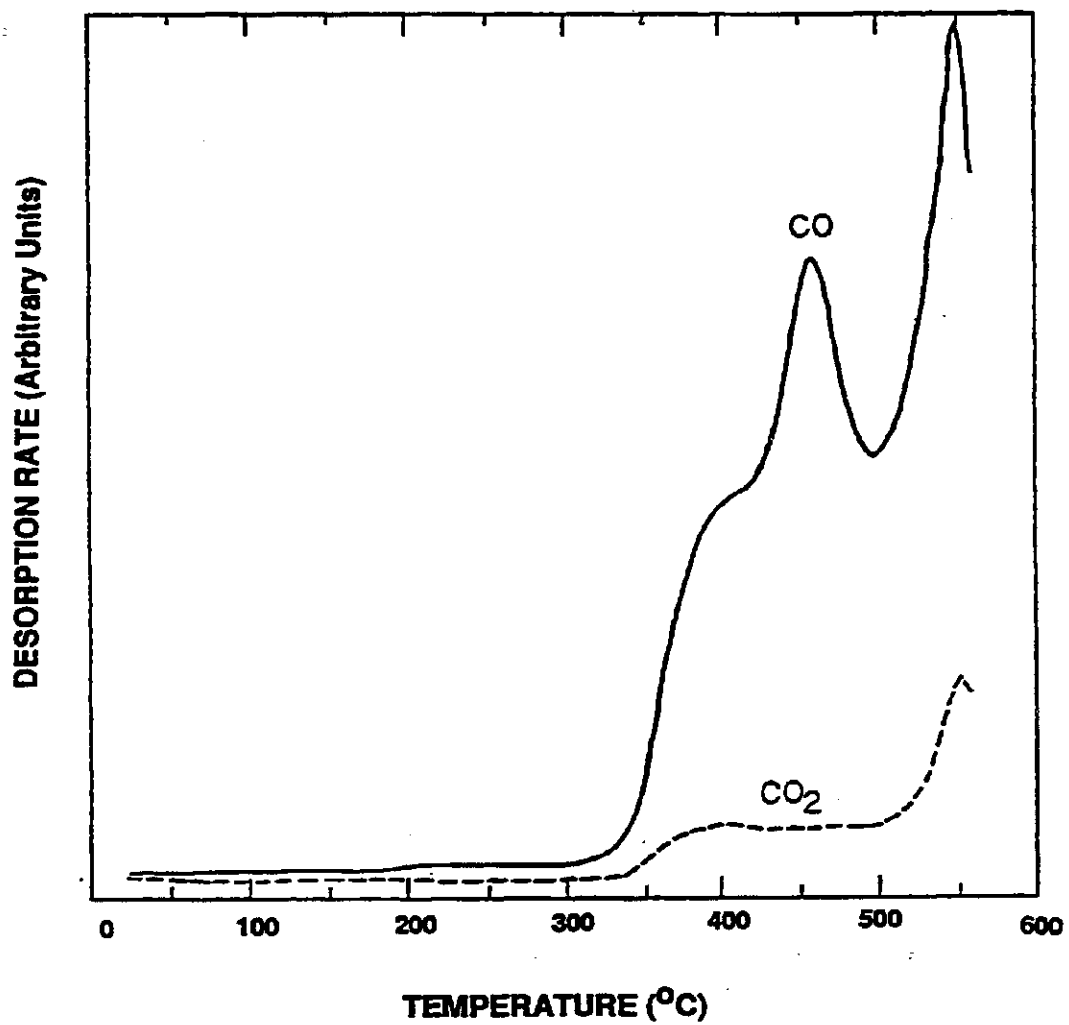


Figure 9. Temperature-programmed desorption spectra of CO and CO₂ from CoB-250 (CO adsorbed at 25 °C).

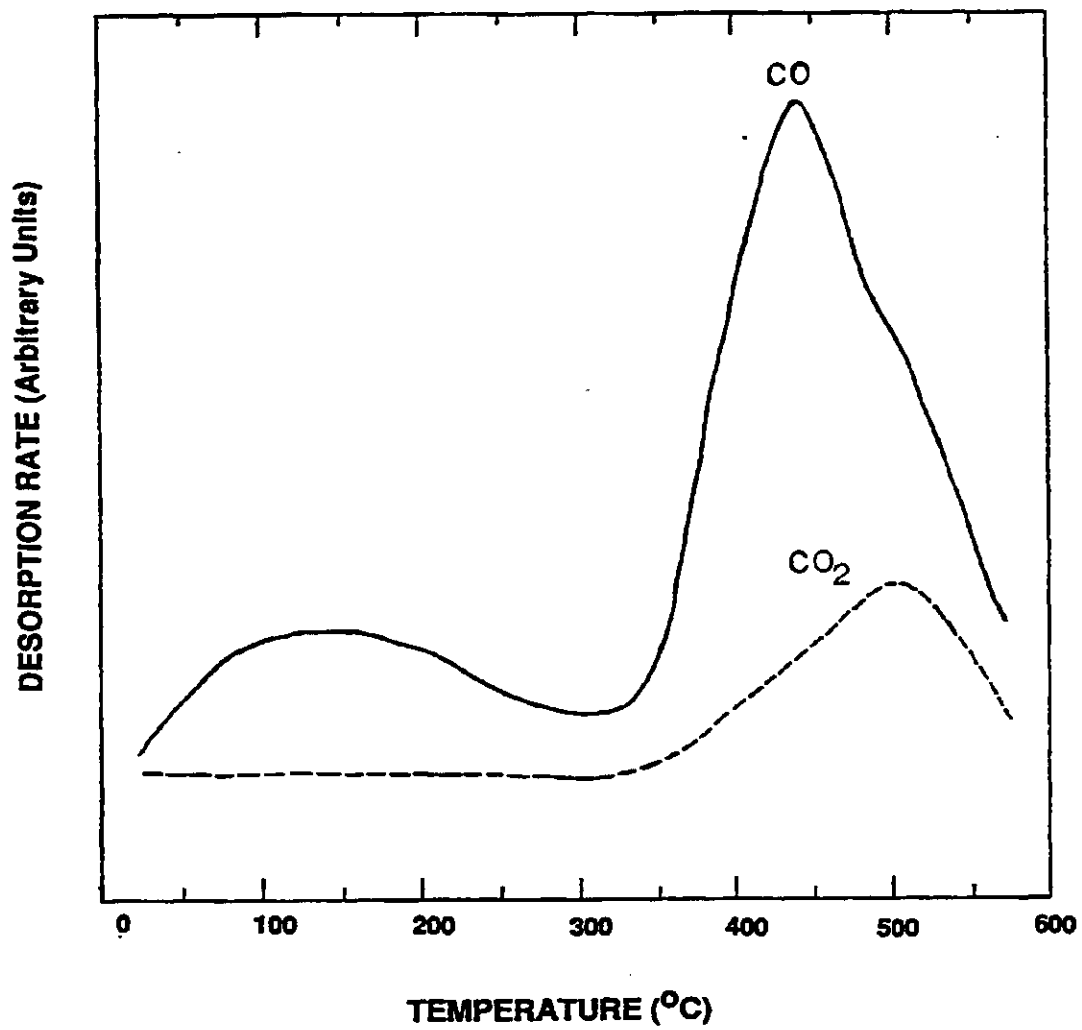


Figure 10. Temperature-programmed desorption spectra of CO and CO₂ from CoB/Na-250 (CO adsorbed at 25 °C).

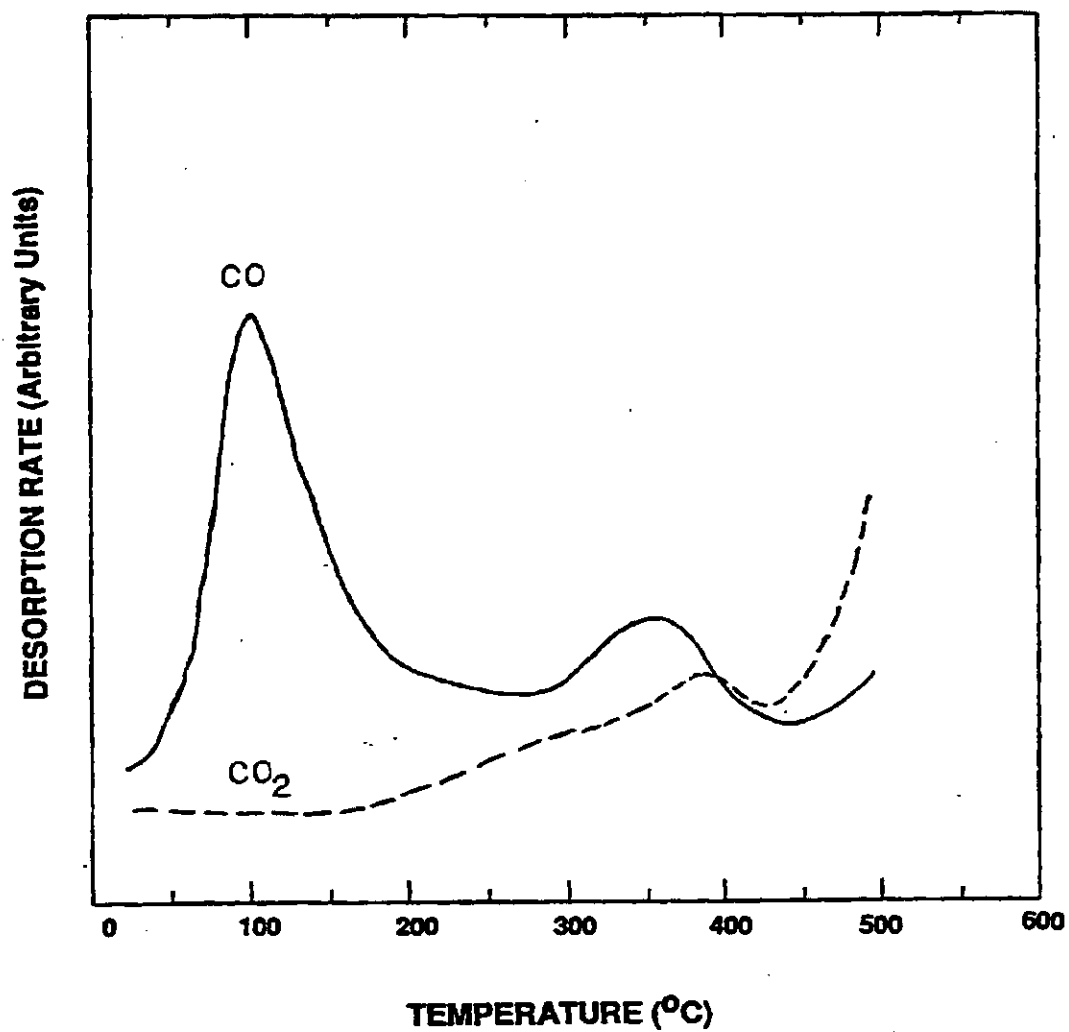


Figure 11. Temperature-programmed desorption spectra of CO and CO₂ from 3% Co/Al₂O₃ (CO adsorbed at 25 °C).

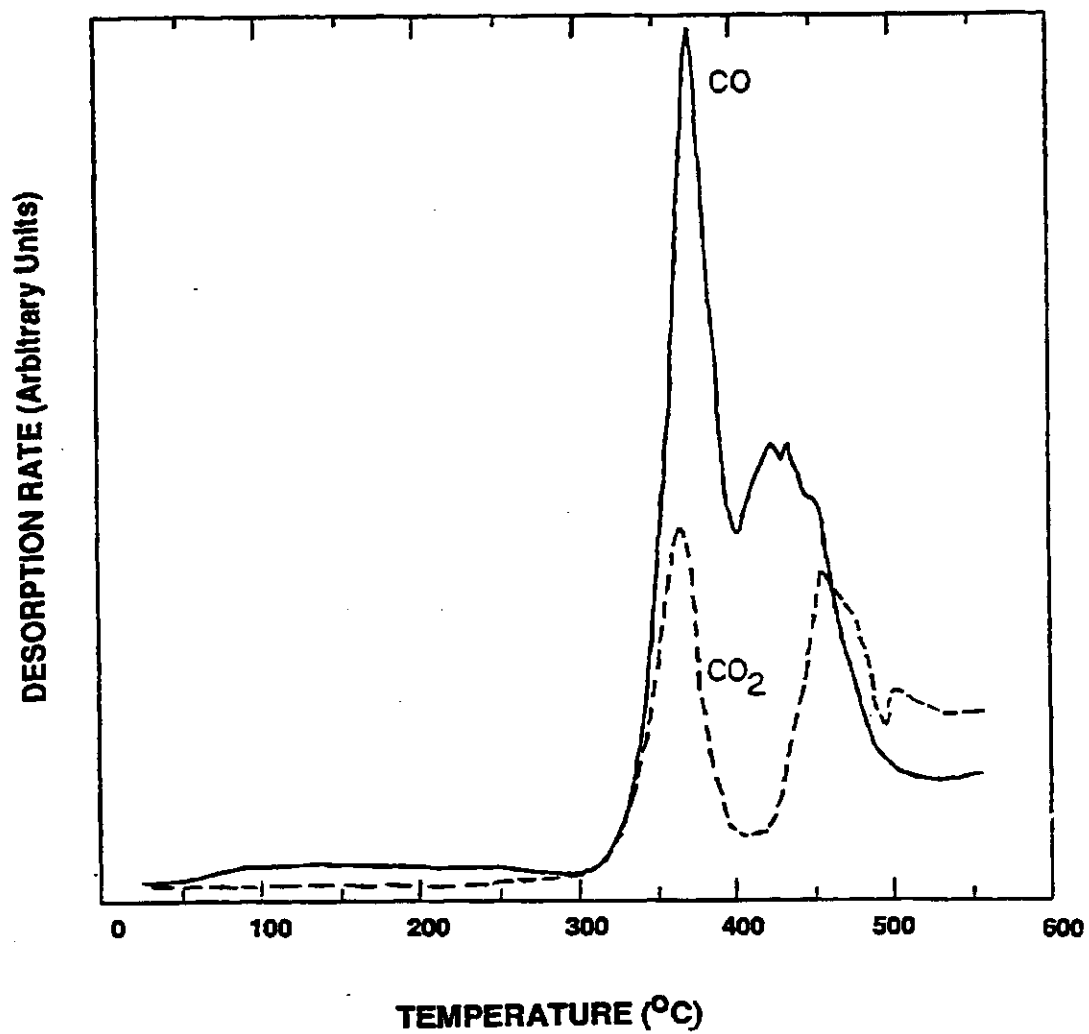


Figure 12. Temperature-programmed desorption spectra of CO and CO₂ from CoB/Al₂O₃-250 (CO adsorbed at 25 °C).

B. Task 2: Activity/Selectivity Measurements

1. High Pressure Reactor System and Chromatographic Analysis. During the first year our analysis of Fischer-Tropsch products was improved with the installation of new columns for separating both hydrocarbons and fixed gases: (i) a 30 meter capillary column coated with OV101 for separating the hydrocarbons (Supelco) and (ii) a 3 meter column packed with Chromosorb-102 (Supelco) for separating fixed gases (e.g. CO, CO₂, CH₄, and H₂).

During the second year, the reactor system for the Fischer-Tropsch Synthesis was modified for operation at pressures up to 400 psig (27 atm). This apparatus is shown schematically in Fig. 1. Hydrogen and carbon monoxide from pressurized cylinders are purified in Deoxo and molecular sieve trap units. The first of two molecular sieve traps for the CO stream is kept at 100°C to remove traces of iron carbonyl from the CO cylinder. Brooks automatic flow controllers are used to control and meter H₂ and CO flows. Heating of the stainless steel reactor is achieved by a tubular, nichrome-wire-wrapped furnace. Pressure in the reactor system is controlled by a Tescom back pressure regulator at the end of the reactor line. A reactor bypass line is provided for convenient reactant sampling. The product stream from the reactor can be routed by a 3-way valve either into a cold trap for the collection of water and higher hydrocarbons to avoid fouling of lines and gas chromatograph sampling system or directly to the G.C. sampling valve for online analysis of the entire spectrum of products. All the lines connecting the reactor to the cold trap and through the G.C. sampling valve are heated by electrical heating elements to avoid condensation of higher molecular weight hydrocarbon products.

2. Experimental Measurements. During the first year CO hydrogenation activity/selectivity tests of unsupported cobalt-boride (Co-B-102), silica-supported cobalt boride (Co-B-S-101) and Fe-B-108 were performed. Specific activity and selectivity data are summarized for the cobalt catalysts in Tables 13 and 14.

The data in Table 13 indicate that the cobalt borides (containing Na) are quite active and stable for CO hydrogen. Indeed, their activities are comparable with those of unpromoted cobalt catalysts (30). Based on the data in Table 14 it is evident that CoB-102 has an unusually high selectivity for C₅₊ hydrocarbons (mostly in the C₅-C₁₂ range), which, nevertheless, decreases with increasing severity of reduction. The selectivity of CoB-S-101 for C₅-C₁₂ hydrocarbons of 49-57% is significantly but not substantially higher than the value of 42% observed for unpromoted Co/SiO₂ (30).

Figure 13 shows the total hydrocarbon product distribution of CoB-102 and the breakdown of olefin and paraffin contributions for each carbon number. This catalyst shows unusually high selectivity for C₅-C₁₂ hydrocarbons as well as C₃-C₇ olefins compared to conventional cobalt catalysts (26). The olefin/paraffin ratio for the product from CoB-S-101 is likewise unusually high compared to a typical cobalt/silica catalyst.

FeB-108 (prepared by NaBH₄ reduction of iron acetate) was also tested and found to deactivate rapidly; its main products were C₂₅-C₃₀ hydrocarbons.

During the second year Co hydrogenation activities and selectivities of 5

Table 13. Specific Activities of Cobalt Borides^a

Catalyst	Reaction Temp. (°C)	Reaction Time (h)	GHSV (h ⁻¹)	CO Conversion (%)	N _{CO} ^b × 10 ³	E _{act} ^c (kJ)
CoB-102	195	37	500	2.62	0.42	140 ^d
	225	--	--	--	3.7	
100% Cobalt ^e	225	6	800	5.0	5.8	95
CoB-S-101	195	46.5	100	1.13	0.21	
	210	34	100	5.34	1.0	163
	225	68	800	2.43	3.6	
	240	24.5	1400	3.18	8.4	
10% Co/SiO ₂ ^e	225	6	--	--	7.5	69

^aAt H₂/CO=2, 1 atm

^bCO turnover frequency, the number of CO molecules converted per second per catalytic site as measured by H₂ adsorption.

^cActivation energy for CO conversion.

^dFrom Ref. 11.

^eData from Ref. 25.

Table 14. Product Selectivities (Weight Fractions)
for CoB-102 and Co-S-101 ($H_2/CO=2$, 1 atm)

Catalyst	Reaction Temp. (°C)	GHSV(h^{-1})	Wt.% Selectivity				
			CH ₄	C ₂ -C ₄	C ₅ -C ₁₃	C ₁₃ ⁺	CO ₂
CoB-102	195 ^a	200	0.3	0.0	97.4	0.0	2.6
	210 ^a	200	0.1	0.1	99.6	0.0	0.2
	225 ^a	500	2.0	4.2	92.5	0.0	1.4
	195 ^b	300	3.6	18.4	75.0	0.0	3.0
	207 ^b	300	3.7	15.2	68.6	0.0	12.5
	223 ^b	300	1.7	11.7	63.1	0.0	23.6
	195 ^c	500	6.2	17.9	59.6	0.0	16.3
100% Co ^d	225	--	29	42	28	0.0	0.0
CoB-S-101	195 ^c	100	18.9	24.2	52.0	0.0	4.9
	210 ^c	100	18.6	24.5	53.3	0.0	3.5
	225 ^c	800	15.7	22.3	57.2	0.0	4.9
	240 ^c	1400	20.3	25.8	48.5	0.0	5.4
10% Co/SiO ₂ ^d	225	800	29	27	42	0.2	0.0

^aReduced at 250°C for 2 hours. Run for 6, 8, 4 hours; data from previous report (Ref. 22).

^bReduced at 250°C for 5 hours. Run for 24, 24 and 30 hours respectively; new data.

^cReduced at 200°C for 5 hours and 250°C for 15 hours. Run for reaction times shown in Table 6.

^dData from Ref. 25.

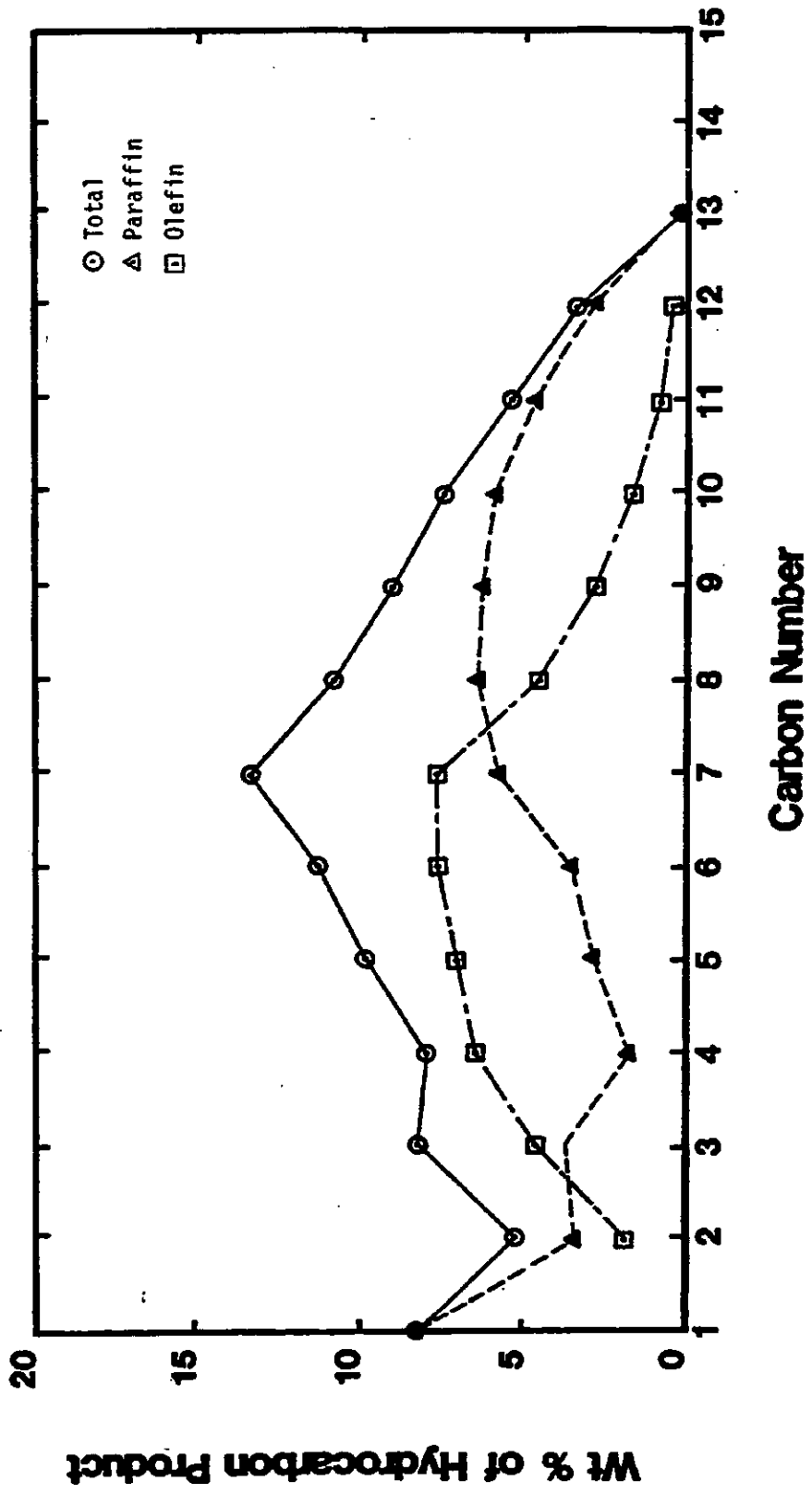


Figure 13. Hydrocarbon product distribution for CoB-102 #8 during CO hydrogenation ($H_2/CO=2$, $T=1950C$, 1 atm).

catalysts, Co-103 (#1), CoB-109 (prepared by gas phase boriding), Co/Na-S-100 (#1), CoB-102 (#9, #10, #11, prepared from NaBH_4), and CoB-A-102 were measured at different temperatures. Activity and selectivity data are summarized for these catalysts in Tables 15 and 16.

Samples of CoB-102, #9 and #11, reduced 15 hours at 250°C and 350°C respectively were tested each at 4 different temperatures (see Table 15). The data in Table 15 show a trend of increasing methane and $\text{C}_2\text{-C}_4$ makes and decreasing C_5+ make with increasing reduction temperature. Unusually high selectivities for $\text{C}_5\text{-C}_{13}$ hydrocarbon products and for $\text{C}_3\text{-C}_8$ olefins were observed for both catalysts. Both catalysts were quite stable and did not lose more than 5% activity over a period of 50-100 hours.

Sodium-free, boron-promoted cobalt (CoB-109) has the same order of magnitude of activity as unpromoted cobalt (Co-103) within experimental error while Na-promoted cobalt is significantly less active (see Table 16). However, CoB-102 (#10) prepared from NaBH_4 reduction and which contains both boron and sodium is a factor of two more active than unpromoted cobalt; in other words, there appear to be a synergistic effect in the case of dual promotion. The cobalt boride catalyst, CoB-109, prepared by gas phase boriding, produces significantly lighter products and has a significantly higher methane make compared to unpromoted cobalt Co-103. The sodium-promoted cobalt/silica, on the other hand, produces significantly more C_{12+} liquids and alcohols relative to unpromoted Co/silica (23). The sodium-promoted cobalt boride (CoB-102, #10) reduced 16 hours at 350°C has a product distribution very similar to that of the unsupported cobalt (Co-103); however, the CoB-102 produces significantly less methane and slightly more $\text{C}_5\text{-C}_{11}$ gasoline range hydrocarbons, especially at lower reduction times (see Table 15).

Unusually high activity and selectivity for C_5+ hydrocarbons, mostly in the range of $\text{C}_5\text{-C}_{11}$ was observed for CoB-A-102 at 210°C (see Table 16). A small fraction of alcohol products was also observed and the selectivity to CO_2 was quite low as in other cobalt borides (CoB-102, #10, #11, and CoB-109). The run with this catalyst was terminated early because the temperature of the catalyst bed increased uncontrollably after the temperature was raised to 225°C. This is probably a result of the high activity of this catalyst leading to adiabatic ignition under these conditions.

During the ninth quarter CO hydrogenation activities and selectivities of 2 catalysts, CoB-105 and CoB-102, were measured at high pressures. The run with CoB-105 (prepared from NaBH_4 in aqueous solution and reduced at 250°C for 15 hours) was unsuccessful as no activity was observed even after the temperature was raised to 250°C at 14 atm. A sample of CoB-102 (prepared from NaBH_4 in ethanolic solution and reduced at 250°C for 15 hours) was tested at 6 atm and 2 different temperatures. Figure 14 shows the total hydrocarbon product distributions of CoB-102 at 1 atm and 6 atm. The data in Figure 14 and Table 17 indicate a trend of increasing methane and $\text{C}_2\text{-C}_4$ makes with increasing pressure at the expense of CO_2 formation; unusually high selectivities for $\text{C}_5\text{-C}_{12}$ hydrocarbon products were observed at both pressures.

Figure 15 shows the total hydrocarbon product distribution of CoB-102 and the breakdown of olefin, and isoparaffin contributions for each carbon number at 6 atm and 196°C. The separation of olefins and branched isomers within a carbon number group was also possible in these experiments. This catalyst

Table 15. Specific Activities and Product Selectivities of CoB-102 Samples Reduced at 250 and 350°C during CO Hydrogenation at $H_2/CO = 2$.

Catalyst I.D. Code	Run No.	Reaction Temp. (°C)	Reaction Time (hr)	% CO Conversion	N_{CO}^a mol/site sec $\times 10^4$	Product Selectivity (wt.%) ^b			Propagation ^c Probability	E_{act}^d (kJ/mol) $\times 10^2$	
						CH ₄	C ₂ -C ₄	C ₅₊			
CoB-102	9 ^e	195	53.0	1.61	0.66	7.4	23.2	55.0	14.4	0.77	159
		210	49.5	8.27	3.4	7.4	18.2	62.3	12.1	0.84	
		225	50.5	7.19	8.8	8.0	19.4	66.1	6.5	0.69	
		240	27.0	12.55	26.	13.1	21.8	55.5	9.6	0.71	
CoB-102	11 ^f	190	43.5	0.62	0.73	10.5	28.9	57.4	3.1	0.74	136
		210	52.0	2.03	2.4	13.8	27.6	55.6	2.9	0.79/0.58	
		225	41.0	2.64	9.4	16.0	27.1	53.0	3.9	0.81/0.55	
		240	32.0	2.55	21.	17.5	28.0	49.5	5.0	0.78/0.58	

^a Turnover frequency, the number of CO molecules reacted per catalytic site per second.

^b Weight percentage of carbon containing products.

^c The slope of $\ln (wt.\%/n)$ versus carbon number.

^d The energy of activation for CO conversion determined from a plot the log of the CO turnover frequency versus reciprocal temperature.

^e Reduced at 250°C in H₂ for 15 hours.

^f Reduced at 350°C in H₂ for 15 hours.

Table 16 Steady-State CO Hydrogenation Activities and Selectivities of Cobalt Catalysts

Catalyst	Run No.	Reaction Temperature (°C)	Reaction Time (hr.)	% CO Conversion	$\text{H}_2\text{O}^a \times 10^3$ Molecules/Site Sec.	Product Selectivity (wt.%)						Propagation Probability α	E_{act} (kJ/mole)
						CH ₄	C ₂ -C ₄	C ₅ -C ₁₁	C ₁₂ ⁺	Alcohols	CO ₂		
Co-103	1	195	55.0	15.64	1.4	12.6	19.4	46.2	18.3	--	3.6	0.82	72
		210	21.0	14.38	3.0	20.0	25.9	39.2	11.0	--	4.0	0.72	
		225	26.0	16.44	4.6	31.0	30.0	26.9	6.1	--	6.0	0.62	
		240	20.0	19.00	7.2	35.4	30.8	20.3	5.1	--	8.4	0.54	
CoB-109	1	212	28	1.94	1.1	35.4	31.9	28.5	--	--	4.2	2.58	118
		225	22	4.76	2.7	40.2	34.1	21.5	--	--	4.2	0.52	
		240	22	10.59	5.5	54.8	30.5	11.2	--	--	3.5	0.44	
		195	43.5	0.76	0.07	12.9	23.2	25.7	5.4	--	32.9	0.72	
Co/Na-S-100	1	210	27.5	1.64	0.16	12.8	22.5	21.4	3.4	--	39.8	0.67	102
		225	10.5	3.95	0.39	12.8	20.6	16.1	4.0	4.3	42.1	0.70	
		240	12.0	7.34	0.72	12.3	18.1	13.3	3.4	3.0	50.0	0.71	
		195	49.0	8.12	2.1	10.7	18.0	48.9	18.0	0.7	3.6	0.79	
CoB-102	10	210	19.0	10.05	6.7	18.0	24.9	42.7	8.9	0.9	4.6	0.70	68
		225	40.0	7.72	7.4	19.7	26.2	36.1	9.6	0.5	7.9	0.68	
		240	14.5	9.86	11.0	27.9	28.4	25.8	5.6	0.3	12.0	0.64	
		210	20	15.7	4.3	14.7	14.7	63.0	4.5	1.5	1.6	1.6	

^aCO turnover frequency CO molecules converted per catalytic site per second.

Table 17. CO Hydrogenation Activities and Selectivities
of Cobalt Boride Catalysts

Catalyst I.D. Code	Run No.	Reaction Temperature (°C)	Reaction Pressure (atm)	Reaction Time (hr.)	% CO Conversion molecule/site sec.	$H_2O \times 10^3$ ^a	Product Selectivity (wt.%) ^b					Propagation ^c Probability	
							C ₁	C ₂ -C ₄	C ₅ -C ₁₁	C ₁₂ ⁺	CO ₂		Alcohols
CoB-A-102		195	1	37	2.62	0.42	6.2	17.9	59.6	0	16.3	0	0.93 (0.66)
CoB-105	19	196	6	15	9.73	0.90	10.9	27.7	58.0	0.5	2.5	0.5	0.78
CoB-102	23	208	6	30	7.84	0.73	12.4	28.0	54.2	0.8	3.3	1.3	0.75

^a Turnover frequency, the number of CO molecules converted per catalytic site (measured by H₂ adsorption) per second.

^b Wt. % of carbon-containing product.

^c The slope of ln (M_n) vs. carbon number.

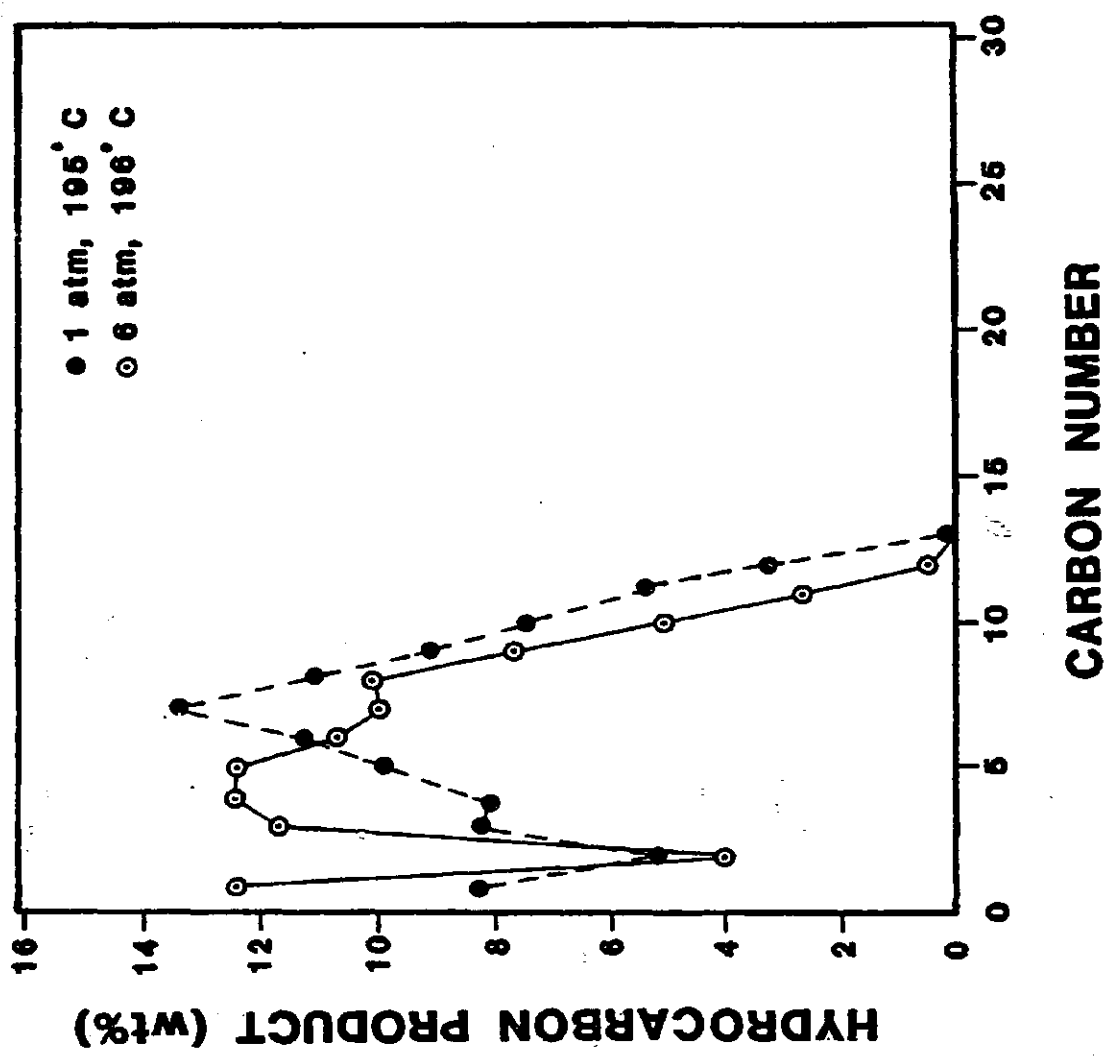


Fig. 14. Hydrocarbon product distribution for CoB-102, H₂/CO = 2.

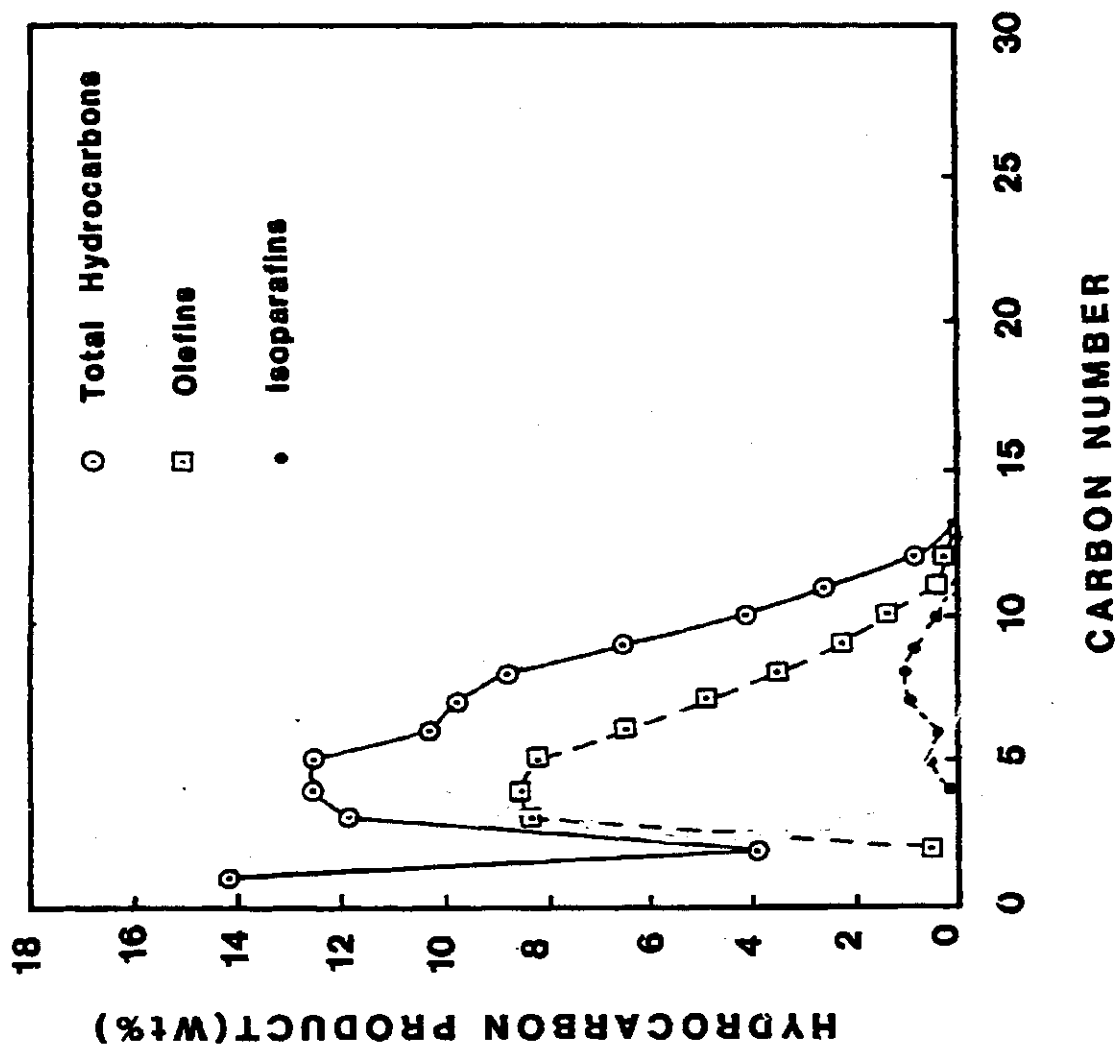


Fig. 16. Hydrocarbon product distribution for CoB-102 at 6 atm, 208°C, H₂/CO = 2.

is highly selective for C_3 - C_8 olefins. Small amounts of isoparaffins (5 wt.%) and alcohols (0.5 wt.%) were also observed. Isoparaffins and higher alcohols are octane boosters for gasoline. A very small amount of solid waxy material, found in the reactor after the run, might account for a deviation of C_{10+} products from the A-S-F model.

During tests at 6 atm, the CO turnover number decreased with increasing temperature as shown in Table 17, suggesting that the catalyst deactivated at the higher temperature, while in previous experiments [26] with CoB-102 at 1 atm, the catalyst was observed to be stable during tests at 195-240°C over periods of 15-40 hours.

During the 10th quarter modifications were made to the reactor system to facilitate online sampling while avoiding trapping of liquids. While making these modifications, it was found that a portion of the line from the G.C. sampling valve to the capillary column (FID) was exposed to ambient room temperature. This probably explains why the product distribution analyzed by G.C. in previous runs was generally cut off sharply at C_{12} or C_{13} .

During the previous quarter it was also found that a small amount of waxy material remained in the reactor during a test of CoB-102. The waxy material collected from this run was analyzed during this quarter by capillary G.C. and was found to contain liquid and waxy hydrocarbons ranging from C_{11} to above C_{30} .

During the 11th quarter CO hydrogenation activities and selectivities of cobalt (Co-104) and cobalt boride (CoB-250) catalysts (the former catalyst reduced at 400°C and the latter catalyst reduced 16 hours at 250°C or 350°C) were measured at different temperatures and pressures. The two cobalt boride samples were each tested at four different temperatures and several different pressures. Activity and selectivity data are summarized for these catalysts in Tables 18-20 while representative hydrocarbon product distributions and Anderson-Schulz-Flory plots are presented in Figures 16 and 17. Comparison of the data for the cobalt boride catalysts in Tables 18 and 19 indicates that at 1 atm, the CoB catalyst reduced at 350°C has higher selectivities for methane and C_2 - C_4 products. At higher pressures (21 atm), the C_5 - C_{11} hydrocarbon product fraction and α values increase as expected for the CoB catalyst reduced at 350°C. However, for the CoB catalyst reduced at 250°C, the C_5 - C_{11} hydrocarbon products decreased slightly at higher pressure. In comparison with the unsupported cobalt catalyst (Table 20), the CoB catalyst tested at 1 atm and reduced at 250°C (Table 18) has a higher selectivity for C_5 - C_{11} products, slightly higher than methane make, and about the same values of α , whereas the CoB catalyst reduced at 350°C (Table 19) has much lower selectivity for C_5 - C_{11} hydrocarbon products, much higher methane make, and significantly lower values of α than the cobalt catalyst. At 21 atm, the CoB catalyst reduced either at 250°C or 350°C has higher selectivity for C_5 - C_{11} range products than observed for conventional cobalt catalysts. It is interesting but unexpected that the polymerization probability of cobalt decreases with increasing pressure.

In general, the CoB catalyst was found to be very active compared to the cobalt catalyst at the same temperature, i.e., a factor ten more active. The specific activities for the CoB catalyst reduced at 250°C are about twice those for the same catalyst reduced at 350°C.

Table 18. Specific Activities and Product Selectivities of Cobalt Boride (Reduced at 250°C) for Steady-State CO Hydrogenation at Different Pressures.

Run No.	Reaction Pressure (atm)	Reaction Temperature °C	Reaction Time (hrs)	% CO Conversion	N _{CO} × 10 ³	Carbon Atom ^b		Product Selectivity					Propag. Probability ^a	Exct. (kJ/mole)
						CO ₂	H.C.	C ₁	C ₂ -C ₄	C ₅ -C ₁₁	C ₁₂ ⁺	Alcs.		
4	1	156	41	4.91	1.4	1.1	98.9	22.6	19.3	43.9	14.2	0	0.796	95
5	1	168	48	4.51	3.0	1.2	98.8	22.4	21.3	45.3	11.0	0	0.770	
6	1	179	67	4.79	6.0	0.9	99.1	23.2	23.1	45.1	8.6	0	0.746	
7	1	189	78	3.29	8.8	1.1	98.9	29.7	29.9	38.8	1.6	0	0.652	
10	11.2	144	114	5.71	1.6	0.4	99.6	22.3	25.0	41.6	11.1	0	0.764	89
9	11.2	157	90	4.17	2.4	0.8	99.2	24.9	25.5	37.4	12.2	0	0.778	
11	11.2	168	118	3.59	4.8	0.6	99.4	25.1	26.3	35.8	12.8	0	0.788	
12	11.2	179	125	4.34	11.5	0.6	99.4	26.3	26.5	36.4	10.8	0	0.764	
14	21	144	167	7.05	4.1	0.4	99.6	17.4	26.1	41.0	15.5	0	0.745	59
17	21	157	192	5.19	5.2	0.4	99.6	21.8	28.0	39.6	10.6	0	0.761	
18	21	168	197	4.13	8.2	0.5	99.5	23.6	30.1	40.2	6.1	0	0.738	
19	21	179	200	4.65	15.5	0.4	99.6	23.7	30.1	38.6	7.6	0	0.742	

^aCO Turnover frequency defined as CO molecules converted per catalytic site per second.

^bBased on total CO converted.

^cWeight percentage of hydrocarbon groups based on total hydrocarbons in the product.

Table 19. Specific Activities and Product Selectivities of Cobalt Boride (Reduced at 350°C) for Steady-State CO Hydrogenation at Different Pressures.

Run No.	Reaction Pressure (atm)	Reaction Temperature °C	Reaction Time (hrs)	% CO Conversion	H ₂ O × 10 ³	Carbon Atom % ^b		Product Selectivity					Propagation Probability ^a	Eact. (kJ/mole)
						CO ₂	H.C.	C ₁	C ₂ -C ₄	C ₅ -C ₁₁	C ₁₂ ⁺	Alcs.		
21	1	156	88	2.21	1.0	1.9	98.1	39.5	33.0	26.0	1.5	0	0.603	81
22	1	168	110	2.32	1.6	1.5	98.5	40.1	32.6	26.0	1.3	0	0.603	
23	1	179	115	2.41	3.0	1.6	98.4	39.6	33.8	25.9	0.7	0	0.579	
24	1	189	120	2.76	4.9	1.1	98.9	39.2	35.7	24.8	0.3	0	0.521	
25	21	144	156	4.41	1.3	0.7	99.3	27.2	29.5	36.7	5.8	0.8	0.727	80
27	21	157	181	5.06	2.2	0.5	99.5	19.9	28.6	41.8	9.0	0.7	0.744	
28	21	168	191	6.00	4.3	0.5	99.5	20.3	27.6	44.3	7.8	0	0.782	
29	21	179	208	4.70	7.5	0.5	99.5	25.1	26.6	39.3	8.3	0.7	0.769	

^aCO Turnover frequency defined as CO molecules converted per catalytic site per second.

^bBased on total CO converted.

^cHeight percentage of hydrocarbon groups based on total hydrocarbons in the product.