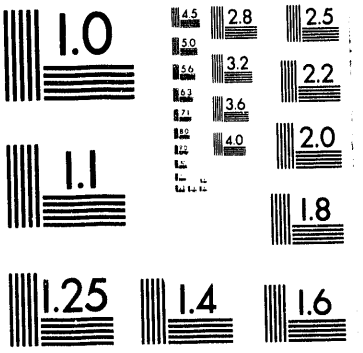
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COPROCESSING THROUGH FUNDAMENTAL AND MECHANISTIC STUDIES IN HYDROGEN TRANSFER AND CATALYSIS

Quarterly Report
for
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MASTER

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Task I. Elucidation of Hydrogen Transfer Reactions in Coprocessing

The objective of this task was to attain a fundamental understanding of the hydrogen transfer reactions that occur during coprocessing and to elucidate their role and importance in achieving upgraded products.

Subtask I.A. Hydrogen Transfer from Cycloalkanes

Introduction

The research conducted this quarter evaluated hydrogen transfer from resids reduced using the Birch reduction method and their corresponding parent resid to an aromatic acceptor, anthracene (ANT). The reactions involved thermal and catalytic reactions using sulfur introduced as thiophenol. This catalyst has been shown by Rudnick[1,2] to affect the hydrogen transfer from cycloalkane to aromatics/or coal.

The purpose of this current study was to evaluate the efficacy of hydrogen transfer from the hydrogen-enriched reduced resid to an aromatic species and to compare that to the hydrogen transfer from the original resid. The analyses performed to evaluate hydrogen transfer were the determination of product slates from the hydrogenation of ANT and the fractionation of the resid into solubility fractions after reaction with ANT.

Three petroleum resids were reduced using the Birch reduction under Task II.C. These reduced resids were reacted in coprocessing reactions with Pittsburgh No. 8 coal. The amount of coal conversion to THF solubles was higher in the coprocessing reactions with the reduced resids compared to the reactions with the corresponding untreated resid. The results from the coprocessing reactions which were reported previously are given in Table 1. The reduction of the resids by the Birch method increased the hydrogen donating ability of the resid to the same

level as that obtained with the introduction of isotetralin (ISO) to the original resid. The ISO was introduced at a level of 0.5 wt. % donable hydrogen.

Both the original resids and the resids reduced by the Birch method were reacted in the presence of an aromatic species, anthracene (ANT). These reactions were performed under both nitrogen and hydrogen atmospheres at a pressure of 1250 psig introduced at ambient temperature. The reactions were performed both thermally and catalytically at 380°C for 30 minutes. The catalyst used was thiophenol which is the same catalyst as has been used in the previously reported model compound studies involving hydrogen transfer from cycloalkanes to aromatics.

Binary Systems of Parent or Reduced Resid with Anthracene Acceptor

Thermal reactions of the parent or reduced resids with ANT under a nitrogen atmosphere and under a hydrogen atmosphere are presented in Tables 2 and 3, respectively. Three different resids were used: Maya, DAU (a deasphalted resid) and S.LA. (a south Louisiana resid). In both nitrogen and hydrogen atmospheres, all of the reduced resids yielded substantially more hydrogenation of ANT than did the parent resids. The hydrogenation products, dihydroanthracene (DHA) and tetrahydroanthracene (THA), were formed. The hydrogen atmosphere promoted more hydrogenation of ANT to these two products than did nitrogen regardless of whether the resid was reduced or not.

Catalytic reactions of the parent and reduced resids with ANT are shown in Table 4. In these experiments, Maya was reacted with ANT under a nitrogen atmosphere while DAU was reacted with ANT under both nitrogen and hydrogen. In the catalytic reactions as with thermal reactions, substantially more conversion of ANT and hydrogenation to DHA and THA occurred

with the reduced resid than with the parent resid. However, the effect of the catalyst for the hydrogenation of ANT was minimal when the thermal and catalytic reactions were compared at equivalent conditions.

The results from the thermal reactions of the various resids with ANT are summarized in Table 5 which gives the percent hydrogenation of ANT. The percent hydrogenation is defined as the moles of hydrogen required to produce the final liquid product as a percentage of the moles of hydrogen required to produce the most hydrogenated product, which is octahydroanthracene in this case. The percent hydrogenation of ANT was greater in hydrogen than in nitrogen. In both atmospheres, the reduced resid hydrogenated more ANT than did the original resid. The individual reduced resids varied in their efficacy. In nitrogen, the reduced resids ranked as DAU > Maya > S.LA., while in hydrogen Maya and DAU were nearly equally effective in transferring hydrogen; both of which were more effective than S.LA. reduced resid.

The product distributions from the resids used in the reactions are given in Tables 6, 7, and 8, where Table 6 is for the reactions under nitrogen, Table 7 is for the reactions under hydrogen and Table 8 is for the catalytic reactions. The resids were fractionated into toluene and tetrahydrofuran solubles. Very little differences were observed among the product distributions from the various reactions. This method of analyzing the resid product was insensitive to the differences among them.

Tertiary Systems With Resid, Anthracene, Perhydropyrene

The tertiary systems involved reacting the reduced or parent resid with perhydropyrene (PHP) and ANT to evaluate the effect of hydrogen transfer from these two resid materials to the

ANT/PHP system. The reactions were performed thermally and catalytically using thiophenol as the catalyst. The resids used were: Maya, DAU (a deasphalted resid) and S.LA. (a south Louisiana resid).

The analyses performed to determine the effect of the reactions on hydrogen transfer were a determination of the products from the model acceptor and donor using gas chromatography and a fractionation of the resid products into oils (hexane solubles), asphaltenes (toluene solubles) and preasphaltenes (tetrahydrofuran solubles). The fractionation analysis of the parent and reduced resids is given in Table 9. The reduced resids tended to have less oils and more asphaltenes and, in the case of Maya, more preasphaltenes and IOM than did the parent resids.

Thermal reactions were performed with the parent resid or reduced resid with PHP and ANT under nitrogen and hydrogen atmospheres. The products achieved from ANT in the nitrogen atmosphere are given in Table 10. For all three resids, substantially more ANT was converted to hydrogenated products, dihydroanthracene (DHA) and tetrahydroanthracene (THA), in the presence of the reduced resid than the parent resid. The reduced Maya and reduced DAU were slightly more effective than the reduced S.LA. The PHP showed ~ 1 to 2% conversion in the different resid systems under nitrogen as shown in Table 11. The products formed were hexahydropyrene (HHP), dihydropyrene (DHP), and pyrene (PYR). The amount of conversion and the products formed were very similar for each parent original and reduced resid system.

More conversion of ANT was observed in the thermal reactions in hydrogen as presented in Table 12 than in the corresponding reactions in nitrogen (Table 10). Once again, the reduced resids showed substantially more hydrogen transfer than did the parent resids. The reduced

Maya and reduced DAU were more active than the reduced S.LA. The PHP reactivity level was very similar in hydrogen to that observed in nitrogen (Table 13).

Catalytic reactions were performed with the resid, PHP, ANT systems. These reactions were performed at 380°C in either nitrogen or hydrogen atmosphere as shown in Table 14. The parent and reduced Maya systems were reacted under nitrogen with 2000 ppm S introduced as thiophenol. The product distributions produced from ANT catalytically were very similar to those produced thermally (Table 10). The catalyst did not seem to promote any additional hydrogen transfer from the resid to ANT under the conditions of the reaction. The catalyst also had little effect on the hydrogen transfer from PHP (Table 15) as compared to the thermal reaction (Table 11).

The Maya original and reduced resid systems were also reacted catalytically in a hydrogen atmosphere. The product distributions achieved from ANT are shown in Table 14 and those from PHP in Table 15. Very little effect of the catalyst was observed in the amount of the products produced compared to the thermal reaction (Table 12). A small positive effect of the catalyst was observed on the reaction of PHP (Table 15) compared to the thermal reactions with hydrogen (Table 13).

A comparison of the effect of the addition of PHP on the hydrogenation of ANT is presented in Tables 16 and 17. In the thermal reactions with nitrogen, the presence of PHP increased the amount of ANT hydrogenation rather substantially. The percentage increase was greater for the parent resid than for the reduced resid. In the thermal reactions in the hydrogen atmosphere, less effect of the PHP was apparent; however, with the original Maya system, the presence of PHP increased the hydrogenation of ANT. In the catalytic reactions, PHP increased

the amount of hydrogenation of ANT in a nitrogen atmosphere for both the original and reduced resids.

Fractionation of Products From Tertiary Systems

The products from the resid were determined by a fractionation of the resid products into oils (hexane solubles), asphaltenes (toluene solubles) and preasphaltenes (tetrahydrofuran solubles). The fractionation analysis of the parent and reduced resids is given in Table 19. The reduced resids had less oils and more asphaltenes and, in the case of Maya, more preasphaltenes and IOM than did the parent resids.

Thermal reactions were performed with the parent resid or reduced resid with PHP and ANT under nitrogen and hydrogen atmospheres. The product distribution for the reactions under nitrogen are given in Table 18 and under hydrogen in Table 19. Comparison of the product distributions from the untreated resids after reactions to those before reaction showed that little change occurred under nitrogen with PHP and ANT present. The parent Maya resid showed an increased oil content and a decreased asphaltene content while DAU parent resid showed the reverse. All of the S.LA. resid was upgraded from asphaltenes to oil. A substantial change was observed in the product distributions of the reduced resid. In all cases, substantial upgrading of the reduced resid to oil occurred, as shown in Figure 1. Similar trends were observed in the reactions with hydrogen except that all of the resids, reduced and parent, showed substantial upgrading from the original materials as shown in Figure 2.

Catalytic reactions using 2000 ppm S introduced as thiophenol were also performed. The product distributions for reactions with parent and reduced resids in nitrogen and hydrogen are given in Table 20. In the nitrogen atmosphere, the upgrading of both the parent and reduced

resid slightly decreased in the catalytic reaction compared to the thermal reactions given in Table 18. A corresponding increase in asphaltenes occurred. In a hydrogen atmosphere, a similar decrease in the oil content and increase in the asphaltene content was observed for both the reduced and parent resids.

Calculation of Hydrogen Transfer to Aromatics from Hydrogen-Rich Species. The results from previously performed hydrogen transfer reaction were calculated in terms of the moles of hydrogen released from the hydrogen donor (Table 22), the percent hydrogenation of aromatics (Table 23), moles of hydrogen used by the hydrogen acceptor (Table 24), hydrogen efficiency (Table 25) and moles of hydrogen from gaseous hydrogen (Table 26). The definitions for these terms are given in Table 21.

A comparison of the moles of hydrogen released from the hydrogen-rich species under conditions where they were introduced at a 1 to 1 and 5 to 1 hydrogen-rich species to aromatic species weight ratio are presented in Table 22 and Figure 3. The reactions with the cyclic olefins, ISO and HHA (hexahydroanthracene), released substantially more hydrogen than the hydroaromatic donors, tetralin (TET) and dihydroanthracene (DHA). The reactions with the cycloalkanes, perhydropyrene (PHP) and perhydroanthracene (PHA), yielded even less moles of hydrogen than did the hydroaromatics. The amount of hydrogen released by the cycloalkanes appeared dependent upon the type of aromatic acceptor present. ANT was able to induce more hydrogen transfer from the cycloalkane PHP than was PYR.

Both the cyclic olefins and the hydroaromatics yielded more hydrogen when the hydrogen donor was present in a 5 to 1 weight ratio of donor to aromatic than in a 1 to 1 weight ratio. However, the ratio did not affect the moles of hydrogen released by the cycloalkane, PHP. The

atmosphere present in the reaction, hydrogen or nitrogen, had very little effect on the amount of hydrogen released from any of the donors.

The amount of hydrogen released from the hydrogen donor had a direct effect on the amount of hydrogenation achieved by the aromatic species. In Table 23, the amount of hydrogenation of ANT and PYR achieved in each of the reactions with the hydrogen donor is presented. Some specific comparisons are given in Figure 4. The most hydrogenation occurred with the cyclic olefins as donors present in a 5 to 1 weight ratio of donor to aromatic. The hydroaromatics yielded the next largest amount of hydrogenation while the cycloalkanes produced the least. ANT hydrogenated more under equivalent reaction conditions than did PYR. The effect of the hydrogen versus the nitrogen atmosphere was dependent upon the type of donor and the acceptor present. In the ISO/ANT system the presence of gaseous hydrogen had little effect on the hydrogenation of ANT while with TET, an ineffective hydrogen donor, the hydrogen atmosphere increased the amount of ANT hydrogenation 20 times. Hydrogen affected the PYR reactions regardless of donor more than the ANT reactions. The hydrogen increased the amount of hydrogenation observed for PYR.

The moles of hydrogen accepted by the hydrogen acceptor are given in Table 24. These moles of hydrogen accepted correlated with the amount of hydrogenation observed in Table 23. The most moles of hydrogen utilized by the PYR system was in the cyclic olefin systems as shown in Figure 5. DHA was a more effective hydroaromatic donor than was TET.

Hydrogen efficiency which is defined as the moles of hydrogen utilized by the aromatic divided by the moles of hydrogen released by the hydrogen donor is presented in Table 25. Some specific cases are illustrated in Figure 6. The hydroaromatic species, particularly DHA,

yielded high hydrogen efficiency in both nitrogen and hydrogen atmospheres while the cyclic olefins yielded low hydrogen efficiency in both atmospheres. The cyclic olefins released substantially more hydrogen than the aromatic compounds were able to utilize under the reaction conditions of 380°C.

In Table 26 and Figures 7 and 8, the moles of hydrogen that came from gaseous hydrogen for the reactions of the hydrogen-rich species with aromatics are presented in two ways. Definition 1, given in Table 27, presents the data as the difference in the moles of hydrogen released compared to the moles of hydrogen accepted. A negative number indicates that more moles of hydrogen were released than utilized. Because the hydrogen released by the hydrogen donor was not completely accepted by the hydrogen acceptor, the first method could not represent the moles of hydrogen from gaseous hydrogen very well. This situation of more moles of hydrogen released than utilized was particularly true for the cyclic olefins.

Definition 2 presents the data as the difference in the moles of hydrogen accepted by the hydrogen acceptor in the hydrogen atmosphere compared to those accepted in a nitrogen atmosphere. This definition provides a more accurate assessment of the quantity of hydrogen coming from gaseous hydrogen. For the PYR systems, the presence of gaseous hydrogen increased the hydrogenation of PYR, particularly when the system was a 5 to 1 weight ratio of hydrogen-rich species to aromatic.

References

1. Rudnick, L. R.; Mobil Oil Corp., USA, "Hydrogenation," Eur. Pat. Appl. EP195539 A2 24 Sep 1986a.

2. Rudnick, L. R.; Mobil Oil Corp., USA, "Conversion of Alicyclic Compounds into Aromatic Compounds," Eur. Pat. Appl. EP195541 A1, 24 Sep 1986.

Table 1. Comparison of Coal Conversion Obtained with Original and Reduced Resids

Reaction	Coal Conversion, %		
	MAYA	DAU	S.LA.
Reduced Resid	43.3	47.0	31.4
Original Resid	20.1	39.6	25.1
Original Resid + ISO	41.5	45.6	33.8

Reaction Conditions: Pittsburgh No. 8 coal, 380°C, 30 minutes

DAU = deasphalted resid S.LA. = south Louisiana resid

Table 2. Product Distributions for Reactions of Anthracene with Various Resids under Nitrogen

Compound/Conditions	Product Distributions, mole %		
	ANT	DHA	THA
MAYA/ANT	87.06(0.68)	11.37(0.73)	1.55(0.06)
MAYA/ANT (Reduced)	67.69(0.55)	26.55(0.49)	5.73(0.07)
DAU/ANT	87.24(0.79)	11.08(0.65)	1.65(0.17)
DAU/ANT (Reduced)	65.27(1.56)	24.04(1.75)	10.67(0.19)
S.LA./ANT	92.28(1.66)	6.77(0.94)	0.93(0.01)
S.LA./ANT (Reduced)	74.43(1.63)	22.13(1.78)	3.42(0.23)

Reaction conditions: 380°C, 1250 psig N_2 charged at ambient conditions.
Number in parentheses indicate standard deviations.

DAU = resid from deasphalting unit
S.LA. = South Louisiana resid
THA = tetrahydroanthracene
ANT = anthracene
DHA = dihydroanthracene

Table 3. Product Distributions for Reactions of Anthracene with Various Resids under Hydrogen

Product Distributions, mole %			
Compound/Conditions	ANT	DHA	THA
MAYA/ANT	75.41(1.56)	21.02(1.42)	3.54(0.14)
MAYA/ANT (Reduced)	46.42(1.98)	35.51(1.19)	18.05(0.81)
DAU/ANT	64.20(1.57)	31.44(1.19)	4.35(0.53)
DAU/ANT (Reduced)	40.81(1.84)	46.56(1.93)	12.61(0.16)
S.LA./ANT	72.42(0.76)	25.99(1.10)	1.57(0.34)
S.LA./ANT (Reduced)	58.51(0.69)	36.00(0.73)	5.47(0.04)

Reaction conditions: 380°C, 1250 psig H_2 charged at ambient conditions.
Number in parentheses indicate standard deviations.

Table 4. Product Distributions for Catalytic Reactions of Anthracene with Various Resids

Product Distributions, mole %			
Compound/Conditions	ANT	DHA	THA
MAYA/ANT (N_2)	86.98(1.23)	11.55(0.95)	1.45(0.30)
MAYA/ANT (Reduced) (N_2)	67.72(0.54)	25.88(0.38)	6.39(0.17)
DAU/ANT (N_2)	85.81(0.38)	12.44(0.37)	1.73(0.16)
DAU/ANT (Reduced) N_2)	64.40(1.29)	26.27(0.94)	9.32(0.38)
DAU/ANT (H_2)	62.55(1.14)	33.04(0.95)	4.40(0.19)
DAU/ANT (Reduced) (H_2)	40.78(0.94)	44.23(0.66)	14.98(0.37)

Reaction conditions: 380°C, 1250 psig H_2 or N_2 charged at ambient conditions.
Number in parentheses indicate standard deviations.

DAU = resid from deasphalting unit
S.LA. = south Louisiana resid
THA = tetrahydroanthracene
ANT = anthracene
DHA = dihydroanthracene

Table 5. Percent Hydrogenation of Reactions of Various Resids with Anthracene

Conditions	H_2	N_2
MAYA/ANT	7.03	3.61
MAYA/ANT (Reduced)	17.90	9.50
DAU/ANT	10.03	3.59
DAU/ANT (Reduced)	17.94	11.34
S.LA./ANT	7.28	2.15
S.LA/ANT (Reduced)	11.73	7.24

DAU = resid from deasphalting resid
S.LA. = south Louisiana resid
ANT = anthracene

Table 6. Product Distributions from Residuum Reactions under Nitrogen

Compound/ Conditions	TOL Solubles %	THF Solubles %	IOM %	Recovery	Conversion %
MAYA/ANT	97.06	2.65	0.27	0.95	99.70
	98.72	0.89	0.38	0.88	99.60
MAYA/ANT (pretreated)	96.25	2.84	0.89	0.82	99.13
	95.66	4.34	0.00	0.84	100.00
DAU/ANT	99.31	0.59	0.08	0.97	99.90
	98.81	1.11	0.07	0.98	99.91
DAU/ANT (pretreated)	98.38	1.41	0.19	0.83	99.80
	95.54	4.33	0.11	0.77	99.89
S.LA./ANT	98.95	0.94	0.10	0.79	99.90
	97.37	2.45	0.18	0.93	99.79
S.LA./ANT (pretreated)	98.26	1.74	0.00	0.87	100.00
	99.02	0.98	0.00	0.76	100.00

Reaction conditions: 380°C, 1250 psig N_2 charged at ambient conditions.

DAU = resid from deasphalting unit
S.LA. = south Louisiana resid
IOM = insoluble organic matter

Table 7. Product Distributions for Residuum Reactions under Hydrogen

Compound/ Conditions	TOL Solubles %	THF Solubles %	IOM %	Recovery	Conversion %
MAYA/ANT	98.60	1.40	0.00	0.98	100.00
	98.90	1.10	0.00	0.97	100.00
MAYA/ANT (pretreated)	98.12	1.48	0.40	0.90	99.52
	98.36	1.31	0.33	0.93	99.60
DAU/ANT	97.08	2.83	0.09	0.86	99.91
	96.64	3.12	0.22	0.98	99.75
DAU/ANT (pretreated)	96.74	3.13	0.11	0.87	99.89
	95.87	3.93	0.20	0.91	99.79
S.LA./ANT	98.88	1.04	0.06	0.96	99.92
	98.48	1.25	0.27	0.87	99.71
S.LA./ANT (pretreated)	97.87	2.00	0.12	0.83	99.88
	98.92	1.08	0.00	0.80	100.00

Reaction conditions: 380°C, 1250 psig H_2 charged at ambient conditions.

ANT = anthracene
DAU = resid from deasphalting unit
S.LA. = south Louisiana resid

IOM = insoluble organic matter
TOL = toluene
THF = tetrahydrofuran

Table 8. Product Distributions for Catalytic Residuum Reactions under Hydrogen

Compound/ Conditions	Atmosphere	TOL Solubles %	THF Solubles %	IOM %	Recovery	Conversion %
MAYA/ANT	N_2	97.98	1.76	0.25	0.98	99.70
Catalytic		98.12	1.83	0.00	0.93	100.00
MAYA/ANT (pretreated)	N_2	99.04	0.79	0.17	0.81	99.84
Catalytic		97.20	2.51	0.29	0.87	99.70
DAU/ANT	N_2	97.10	2.80	0.00	0.83	100.00
Catalytic		96.53	3.10	0.37	0.85	99.63
DAU/ANT (pretreated)	N_2	90.09	3.20	0.69	0.92	99.24
Catalytic		96.82	1.96	1.22	0.85	99.78
DAU/ANT	H_2	96.73	3.27	0.00	0.97	100.00
Catalytic		97.01	2.99	0.00	0.84	100.00
DAU/ANT (pretreated)	H_2	97.96	2.04	0.00	0.92	100.00
Catalytic		97.49	4.51	0.00	0.93	100.00

Reaction conditions: 380°C, 1250 psig H_2 charged at ambient conditions.

DAU = resid from deasphalting unit
ANT = anthracene
IOM = insoluble organic matter
TOL = toluene
THF = tetrahydrofuran

Table 9. Product Distribution of the Resids Before Reaction

Resid	Oil (%)	Asphaltene (%)	Preasphaltene (%)	IOM (%)
MAYA	69.42	30.58	0.00	0.00
Reduced MAYA	35.12	31.18	20.14	13.56
DAU	79.02	20.98	0.00	0.00
Reduced DAU	68.34	31.65	0.00	0.00
S.LA.	95.20	4.80	0.00	0.00
Reduced S.LA.	93.83	6.17	0.00	0.00

DAU = resid from deasphalting unit
S.LA. = South Louisiana resid

Table 10. Reaction Products from Anthracene from Thermal Reactions of Resids with Anthracene and Perhydropyrene under Nitrogen

Compound/Conditions	Product Distributions, mole %		
	ANT	DHA	THA
MAYA/PHP/ANT	74.00(1.43)	24.40(0.46)	1.59(1.83)
MAYA/PHP/ANT (Reduced)	56.27(1.09)	35.28(0.36)	8.43(0.83)
DAU/PHP/ANT	70.53(0.78)	26.83(1.10)	2.63(0.61)
DAU/PHP/ANT (Reduced)	57.24(0.33)	33.25(0.37)	9.50(0.12)
S.LA./PHP/ANT	83.93(1.31)	14.68(1.34)	1.38(0.07)
S.LA./PHP/ANT (Reduced)	59.21(1.30)	36.40(1.43)	4.38(0.18)

Reaction conditions: 380°C, 1250 psig N_2 charged at ambient conditions.
Numbers in parentheses are standard deviations.

ANT = anthracene
THA = tetrahydroanthracene
S.LA. = south Louisiana
DHA = dihydroanthracene
DAU = resid from deasphalting unit

Table 11. Reaction Products from Perhydropyrene from Thermal Reactions of Resids with Anthracene and Perhydropyrene under Nitrogen

Compound/Conditions	Product Distributions, mole %			
	PHP	HHP	DHP	PYR
MAYA/PHP/ANT	97.78(0.22)	0.63(0.06)	0.35(0.27)	1.23(0.07)
MAYA/PHP/ANT (Reduced)	97.94(0.23)	0.47(0.03)	0.64(0.03)	0.94(0.18)
DAU/PHP/ANT	98.96(0.07)	0.39(0.09)	0.49(0.02)	0.15(0.02)
DAU/PHP/ANT (Reduced)	98.76(0.11)	0.54(0.08)	0.49(0.03)	0.20(0.02)
S.LA./PHP/ANT	98.14(0.09)	0.48(0.05)	0.53(0.04)	0.84(0.08)
S.LA./PHP/ANT (Reduced)	98.03(0.07)	0.70(0.07)	0.63(0.03)	0.63(0.05)

Reaction conditions: 380°C, 1250 psig N_2 charged at ambient conditions.
Numbers in parentheses are standard deviations.

PHP = perhydropyrene
DHP = dihydropyrene
DAU = resid from deasphalting unit
HHP = hexahydropyrene
PYR = pyrene
S.LA. = south Louisiana resid

Table 12. Reaction Products from Anthracene from Thermal Reactions of Resids with Anthracene and Perhydropyrene under Hydrogen

Compound/Conditions	Product Distributions, mole %		
	ANT	DHA	THA
MAYA/PHP/ANT	59.47(1.87)	36.61(2.08)	3.90(0.22)
MAYA/PHP/ANT (Reduced)	40.04(0.52)	49.50(1.55)	10.44(1.05)
DAU/PHP/ANT	61.67(1.85)	34.46(1.60)	3.85(0.27)
DAU/PHP/ANT (Reduced)	39.92(0.79)	48.03(0.74)	12.03(0.13)
S.LA./PHP/ANT	74.61(1.37)	23.81(1.24)	1.56(0.16)
S.LA./PHP/ANT (Reduced)	50.45(1.21)	44.38(0.86)	5.27(0.21)

Reaction conditions: 380°C, 1250 psig H_2 charged at ambient conditions.
Numbers in parentheses are standard deviations.

ANT = anthracene
THA = tetrahydroanthracene
S.LA. = south Louisiana resid
DHA = dihydroanthracene
DAU = resid from deasphalting unit

Table 13. Reaction Products from Perhydropyrene from Thermal Reactions of Resids with Anthracene and Perhydropyrene

Compound/Conditions	Product Distributions, mole %			
	PHP	HHP	DHP	PYR
MAYA/PHP/ANT	98.17(0.08)	0.55(0.03)	0.52(0.03)	0.75(0.08)
MAYA/PHP/ANT (Reduced)	98.66(0.12)	0.49(0.03)	0.47(0.08)	0.36(0.05)
DAU/PHP/ANT	99.13(0.03)	0.36(0.07)	0.33(0.04)	0.16(0.00)
DAU/PHP/ANT (Reduced)	98.94(0.20)	0.47(0.18)	0.44(0.07)	0.14(0.09)
S.LA./PHP/ANT	98.29(0.08)	0.44(0.03)	0.59(0.10)	0.68(0.03)
S.LA./PHP/ANT (Reduced)	98.62(0.08)	0.05(0.05)	0.58(0.02)	0.30(0.03)

Reaction conditions: 380°C, 1250 psig H_2 charged at ambient conditions.
Numbers in parentheses are standard deviations.

PHP = perhydropyrene
DHP = dihydropyrene
DAU = resid from deasphalting unit
HHP = hexahydropyrene
PYR = pyrene
S.LA. = south Louisiana resid

Table 14. Reaction Products from Anthracene from Catalytic Reactions of Resids with Anthracene and Perhydropyrene

Compound/Conditions	Product Distributions, mole %		
	ANT	DHA	THA
MAYA/PHP/ANT (N_2)	74.06(0.75)	22.46(0.53)	3.47(0.22)
MAYA/PHP/ANT (Reduced) (N_2)	56.51(1.05)	36.29(1.24)	7.18(0.28)
MAYA/PHP/ANT (H_2)	59.20(1.17)	36.26(1.47)	4.52(0.30)
MAYA/PHP/ANT (Reduced) (H_2)	39.90(0.71)	49.69(0.92)	10.39(0.30)

Reaction conditions: 380°C, 1250 psig H_2 or N_2 charged at ambient conditions, 2000 ppm S introduced as thiophenol.
Numbers in parentheses are standard deviations.

ANT = anthracene
THA = tetrahydroanthracene
DHA = dihydroanthracene
DAU = resid from deasphalting unit

Table 15. Reaction Products from Perhydropyrene from Catalytic Reactions of Resid with Anthracene and Perhydropyrene

Compound/Conditions	Product Distributions, mole %			
	PHP	HHP	DHP	PYR
MAYA/PHP/ANT (N_2)	97.51(0.13)	0.43(0.03)	0.59(0.09)	1.46(0.08)
MAYA/PHP/ANT (Reduced) (N_2)	98.25(0.31)	0.48(0.05)	0.61(0.07)	0.65(0.24)
MAYA/PHP/ANT (H_2)	97.76(0.16)	0.48(0.07)	0.66(0.01)	1.08(0.11)
MAYA/PHP/ANT (Reduced) (H_2)	98.83(0.22)	0.42(0.03)	0.50(0.03)	0.24(0.17)

Reaction conditions: 380°C, 1250 psig H_2 or N_2 charged at ambient conditions.
Numbers in parentheses are standard deviations.

PHP = perhydropyrene
HHP = hexahydropyrene
DHP = dihydropyrene
PYR = pyrene

Table 16. Percent Hydrogenation of Anthracene for Reactions of Various Resids with Anthracene

Condition	H_2	N_2
Thermal		
MAYA/ANT	7.03(0.42)	3.61(0.16)
MAYA/ANT (Reduced)	17.90(0.60)	9.50(0.15)
DAU/ANT	10.03(0.51)	3.60(0.23)
DAU/ANT (Reduced)	17.94(0.44)	11.34(0.34)
S.LA./ANT	7.28(0.11)	2.16(0.24)
S.LA./ANT (Reduced)	11.74(0.17)	7.24(0.38)
Catalytic		
MAYA/ANT		3.61(0.38)
MAYA/ANT (Reduced)		9.66(0.18)
DAU/ANT	10.46(0.33)	3.99(0.11)
DAU/ANT (Reduced)	18.54(0.32)	11.23(0.41)

DAU = resid form deasphalting unit
S.LA. = South Louisiana resid

Table 17. Percent Hydrogenation of Anthracene for Reactions of Various Resids with Perhydropyrene and Anthracene

Condition	H_2	N_2
Thermal		
MAYA/PHP/ANT	11.10(0.42)	6.90(0.81)
MAYA/PHP/ANT (Reduced)	17.60(0.15)	13.03(0.47)
DAU/PHP/ANT	10.54(0.52)	8.02(0.21)
DAU/PHP/ANT (Reduced)	18.02(0.22)	13.06(0.08)
S.LA./PHP/ANT	6.73(0.38)	4.36(0.31)
S.LA./PHP/ANT (Reduced)	13.73(0.32)	11.29(0.29)
Catalytic		
MAYA/PHP/ANT	11.33(0.21)	7.11(0.24)
MAYA/PHP/ANT (Reduced)	17.62(0.14)	12.66(0.22)

DAU = resid from deasphalting unit
S.LA. = South Louisiana resid

Table 18. Product Distributions for Thermal Reactions in Nitrogen

Resid	Oil (%)	Asphaltenes (%)	Preasphaltenes (%)	IOM (%)
MAYA/PHP/ANT	73.67(0.91)	26.33(0.91)	0.00(0.00)	0.00(0.00)
Reduced MAYA/PHP/ANT	81.92(0.00)	18.08(0.00)	0.00(0.00)	0.00(0.00)
DAU/PHP/ANT	76.55(0.62)	23.44(0.63)	0.00(0.00)	0.00(0.00)
Reduced DAU/PHP/ANT	83.02(0.31)	16.97(0.30)	0.00(0.00)	0.00(0.00)
S.LA./PHP/ANT	100.00(0.00)	0.00(0.00)	0.00(0.00)	0.00(0.00)
Reduced S.LA./PHP/ANT	100.00(0.00)	0.00(0.00)	0.00(0.00)	0.00(0.00)

Table 19. Product Distributions for Thermal Reactions in Hydrogen

Resid	Oil (%)	Asphaltenes (%)	Preasphaltenes (%)	IOM (%)
MAYA/PHP/ANT	76.83(1.16)	23.16(1.17)	0.00(0.00)	0.00(0.00)
Reduced MAYA/PHP/ANT	78.08(2.05)	21.90(2.05)	0.00(0.00)	0.00(0.00)
DAU/PHP/ANT	81.14(1.40)	18.85(1.40)	0.00(0.00)	0.00(0.00)
Reduced DAU/PHP/ANT	88.38(6.09)	11.61(6.09)	0.00(0.00)	0.00(0.00)
S.LA./PHP/ANT	100.00(0.00)	0.00(0.00)	0.00(0.00)	0.00(0.00)
Reduced S.LA./PHP/ANT	100.00(0.00)	0.00(0.00)	0.00(0.00)	0.00(0.00)

DAU = resid from deasphalting unit

S.LA. = south Louisiana resid

Numbers in parentheses indicate standard deviations.

Table 20. Product Distributions for Catalytic Resid Reactions

Compound/Conditions	Oil (%)	Asphaltenes (%)	Preasphaltenes (%)	IOM (%)
MAYA/PHP/ANT (N_2)	70.02(1.40)	29.97(1.40)	0.00(0.00)	0.00(0.00)
MAYA/PHP/ANT (Reduced) (N_2)	80.79(2.21)	19.20(2.21)	0.00(0.00)	0.00(0.00)
MAYA/PHP/AND (H_2)	74.14(0.90)	25.85(0.90)	0.00(0.00)	0.00(0.00)
MAYA/PHP/ANT (Reduced) (H_2)	75.79(1.11)	24.20(1.11)	0.00(0.00)	0.00(0.00)

Reaction conditions: 380°C, 1250 psig H_2 or N_2 charged at ambient conditions.

Numbers in parentheses indicate standard deviations.

Table 21. Definitions of Calculated Terms

Percent Hydrogenation

Moles of hydrogen required to achieve the liquid products as a percentage of the moles of hydrogen needed to produce the most hydrogenated product.

Calculation of Moles of Hydrogen Used by a Hydrogen Acceptor

(Moles of hydrogen accepted by the hydrogen acceptor) = (moles of product x moles of hydrogen used)

Calculation of Moles of Hydrogen Released from Hydrogen Donor

(Moles of hydrogen released from the hydrogen donor) = (hydrogen released from the hydrogen donor - hydrogen used by the hydrogen donor) = (moles of product x moles of hydrogen released) - (moles of product x moles of hydrogen used)

Calculation of Hydrogen Efficiency

Hydrogen efficiency = (moles of hydrogen accepted by the hydrogen acceptor) divided by (moles of hydrogen released by the hydrogen donor)

Calculation of the Amount of Gaseous Hydrogen that was Accepted by Hydrogen Acceptor

I. Amount of hydrogen accepted that came from gaseous hydrogen = moles of hydrogen accepted by hydrogen acceptor - moles of hydrogen released from the donor.

II. Amount of hydrogen accepted that came from gaseous hydrogen = moles of hydrogen accepted by hydrogen acceptor under a hydrogen atmosphere - moles of hydrogen accepted by hydrogen acceptor under a nitrogen atmosphere.

Table 22. Moles of Hydrogen Released from the Hydrogen Donor

Condition	Moles of Hydrogen Released * 10^4	
	H_2 Atmosphere	N_2 Atmosphere
ISO	10.73(0.17)	11.39(0.06)
ISO/ANT (1:1)	11.08(0.03)	17.00(0.06)
ISO/ANT (5:1)	44.69(0.61)	45.42(0.13)
TET	0.05(0.03)	0.03(0.00)
TET/ANT (1:1)	0.05(0.02)	0.00(0.00)
TET/ANT (5:1)	0.11(0.03)	0.39(0.03)
PHP	0.00(0.00)	0.00(0.00)
PHP/ANT (1:1)	0.27(0.02)	0.28(0.05)
PHP/ANT (5:1)	0.18(0.01)	0.25(0.02)
ISO/PYR (1:1)	10.99(0.13)	11.80(0.19)
ISO/PYR (5:1)	49.46(0.79)	47.65(0.32)
TET/PYR (1:1)	0.00(0.00)	0.00(0.00)
TET/PYR (5:1)	0.07(0.00)	0.28(0.19)
HHA	9.95(0.31)	9.95(0.09)
HHA/PYR (1:1)	9.93(0.01)	9.52(0.31)
HHA/PYR (5:1)	35.84(0.48)	43.67(0.82)
DHA	0.35(0.06)	0.28(0.00)
DHA/PYR (1:1)	0.43(0.01)	0.52(0.05)
DHA/PYR (5:1)	1.96(0.03)	1.78(0.19)
PHA	0.00(0.00)	0.00(0.00)
PHA/PYR (1:1)	0.00(0.00)	0.00(0.00)
PHP/PYR (1:1)	0.00(0.00)	0.00(0.00)

ISO = isotetralin
ANT = anthracene
TET = tetralin
PHP = perhydropyrene
PYR = pyrene
HHA = hexahydropyrene
DHA = dihydropyrene
PHA = perhydroanthracene

Table 23. Percent Hydrogenation of Aromatics Obtained in Reactions with Hydrogen-Rich Species*

Condition	Percent Hydrogenation	
	H_2 (%) Atmosphere	N_2 (%) Atmosphere
ISO/ANT (1:1)	19.24(0.27)	18.32(0.14)
ISO/ANT (5:1)	24.88(0.07)	24.39(0.18)
TET/ANT (1:1)	4.53(0.26)	0.25(0.05)
TET/ANT (5:1)	4.45(0.25)	0.93(0.07)
PHP/ANT (1:1)	3.08(0.28)	0.46(0.17)
PHP/ANT (5:1)	3.97(0.42)	0.63(0.02)
ISO/PYR (1:1)	6.02(0.25)	4.11(0.30)
ISO/PYR (5:1)	17.30(0.27)	13.20(0.75)
TET/PYR (1:1)	0.00(0.00)	0.00(0.00)
TET/PYR (5:1)	0.41(0.09)	0.16(0.01)
HHA/PYR (1:1)	13.59(0.23)	8.14(0.84)
HHA/PYR (5:1)	30.35(0.97)	10.40(2.48)
DHA/PYR (1:1)	2.46(0.18)	1.63(0.85)
DHA/PYR (5:1)	11.27(0.35)	8.58(2.17)
PHA/PYR (1:1)	0.34(0.04)	0.29(0.04)
PHA/PYR (5:1)	0.43(0.08)	0.38(0.09)

*For calculation, octahydroanthracene was considered the most hydrogenated liquid product for anthracene and hexahydropyrene was the most hydrogenated liquid product for pyrene.

ISO = isotetralin
ANT = anthracene
TET = tetralin
PHP = perhydropyrene
PYR = pyrene
HHA = hexahydropyrene
DHA = dihydropyrene
PHA = perhydroanthracene

Table 24. Moles of Hydrogen Accepted by the Hydrogen Acceptor

Condition	Moles of Hydrogen Used * 10^4	
	H_2 Atmosphere	N_2 Atmosphere
ISO/ANT (1:1)	4.31(0.06)	4.10(0.03)
ISO/ANT (5:1)	5.58(0.01)	5.46(0.04)
TET/ANT (1:1)	1.01(0.06)	0.05(0.00)
TET/ANT (5:1)	0.99(0.05)	0.21(0.01)
PHP/ANT (1:1)	0.69(0.05)	0.10(0.03)
PHP/ANT (5:1)	0.88(0.09)	0.14(0.00)
ISO/PYR (1:1)	0.88(0.03)	0.60(0.04)
ISO/PYR (5:1)	2.56(0.04)	1.95(0.11)
TET/PYR (1:1)	0.00(0.00)	0.00(0.00)
TET/PRY (5:1)	0.05(0.01)	0.03(0.00)
HHA/PYR (1:1)	2.01(0.03)	1.20(0.12)
HHA/PYR (5:1)	4.49(0.14)	1.54(0.36)
DHA/PYR (1:1)	0.37(0.03)	0.22(0.10)
DHA/PYR (5:1)	1.67(0.05)	1.27(0.32)
PHA/PYR (1:1)	0.04(0.00)	0.03(0.00)
PHA/PYR (5:1)	0.05(0.01)	0.04(0.00)

ISO = isotetralin
ANT = anthracene
TET = tetralin
PHP = perhydropyrene
PYR = pyrene
HHA = hexahydropyrene
DHA = dihydropyrene
PHA = perhydroanthracene

Table 25. Hydrogen Efficiency

Condition	Hydrogen Efficiency	
	H_2 Atmosphere	N_2 Atmosphere
ISO/ANT (1:1)	0.39(0.01)	0.24(0.00)
ISO/ANT (5:1)	0.12(0.00)	0.12(0.00)
TET/ANT (1:1)	19.77(2.89)	---
TET/ANT (5:1)	8.84(1.68)	0.54(0.14)
PHP/ANT (1:1)	2.57(0.22)	0.35(0.09)
PHP/ANT (5:1)	4.91(0.84)	0.57(0.07)
ISO/PYR (1:1)	0.08(0.00)	0.05(0.00)
ISO/PYR (5:1)	0.05(0.00)	0.04(0.00)
TET/PYR (1:1)	---	---
TET/PYR (5:1)	0.79(0.18)	0.17(0.12)
HHA/PYR (1:1)	0.20(0.00)	0.13(0.02)
HHA/PYR (5:1)	0.13(0.01)	0.04(0.01)
DHA/PYR (1:1)	0.87(0.06)	0.44(0.20)
DHA/PYR (5:1)	0.85(0.04)	0.72(0.17)
PHA/PYR (1:1)	---	---
PHA/PYR (5:1)	---	---

* --- means no hydrogen was released in that condition.

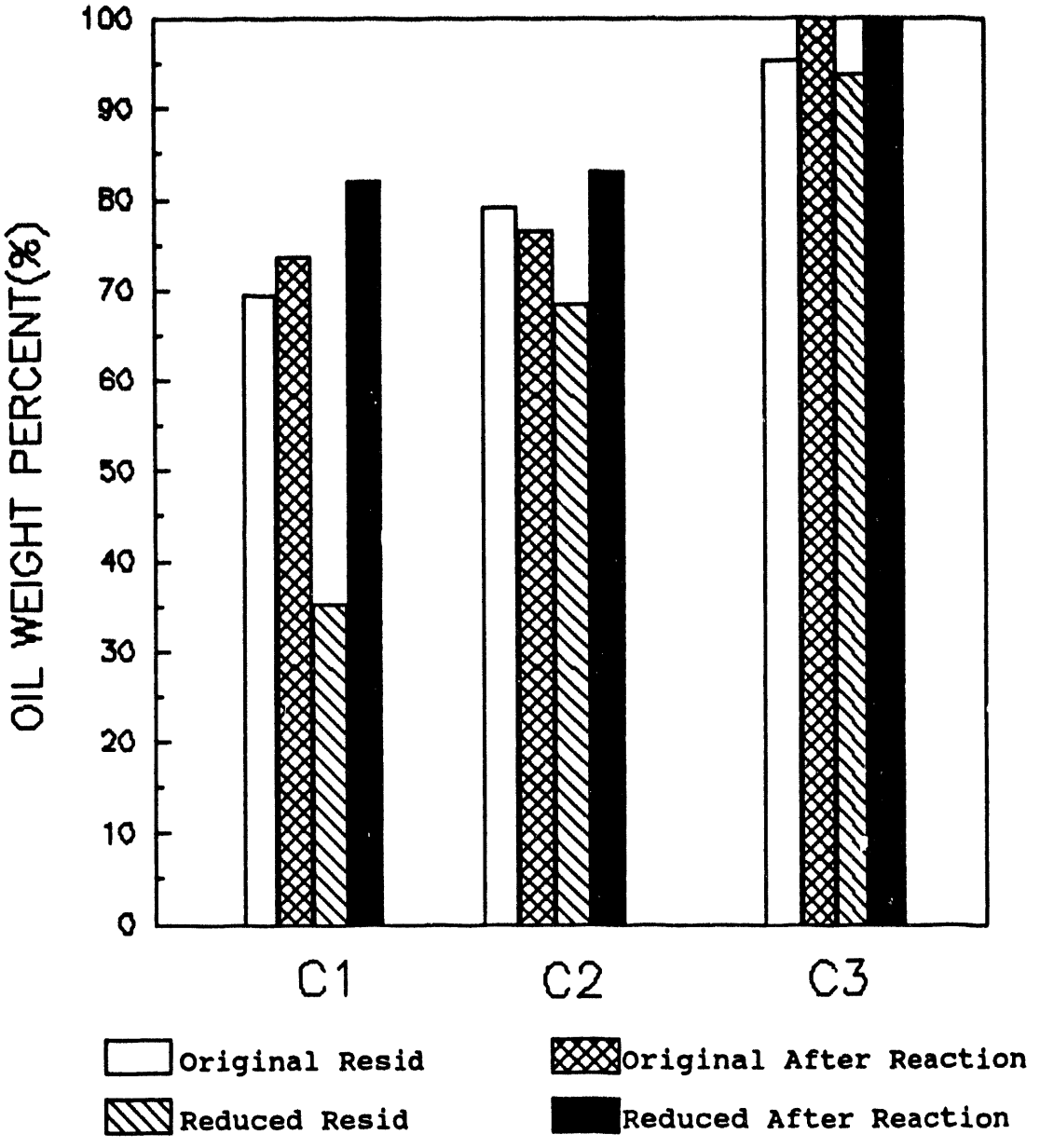
ISO = isotetralin
ANT = anthracene
TET = tetralin
PHP = perhydropyrene
PYR = pyrene
HHA = hexahydropyrene
DHA = dihydropyrene
PHA = perhydroanthracene

Table 26. Moles of Hydrogen from Gaseous Hydrogen

Condition	Definition 1	Definition 2
	H_2 (moles * 10^4)	H_2 (moles * 10^4)
ISO/ANT (1:1)	−10.99(0.13)	0.21(0.09)
ISO/ANT (5:1)	−46.88(0.79)	0.12(0.05)
TET/ANT (1:1)	0.00(0.00)	0.96(0.06)
TET/ANT (5:1)	−0.05(0.02)	0.40(0.08)
PHP/ANT (1:1)	0.41(0.05)	0.59(0.08)
PHP/ANT (5:1)	0.70(0.10)	0.74(0.09)
ISO/PYR (1:1)	−6.76(0.07)	0.28(0.07)
ISO/PYR (5:1)	−39.10(0.59)	0.61(0.15)
TET/PYR (1:1)	0.95(0.05)	0.00(0.00)
TET/PYR (5:1)	0.80(0.00)	0.02(0.01)
HHA/PYR (1:1)	−7.91(0.04)	0.81(0.15)
HHA/PYR (5:1)	−31.33(0.62)	2.95(0.50)
DHA/PYR (1:1)	−0.05(0.02)	0.15(0.13)
DHA/PYR (5:1)	−0.28(0.08)	0.40(0.37)
PHA/PYR (1:1)	0.04(0.00)	0.04(0.00)
PHA/PYR (5:1)	0.05(0.01)	0.05(0.01)

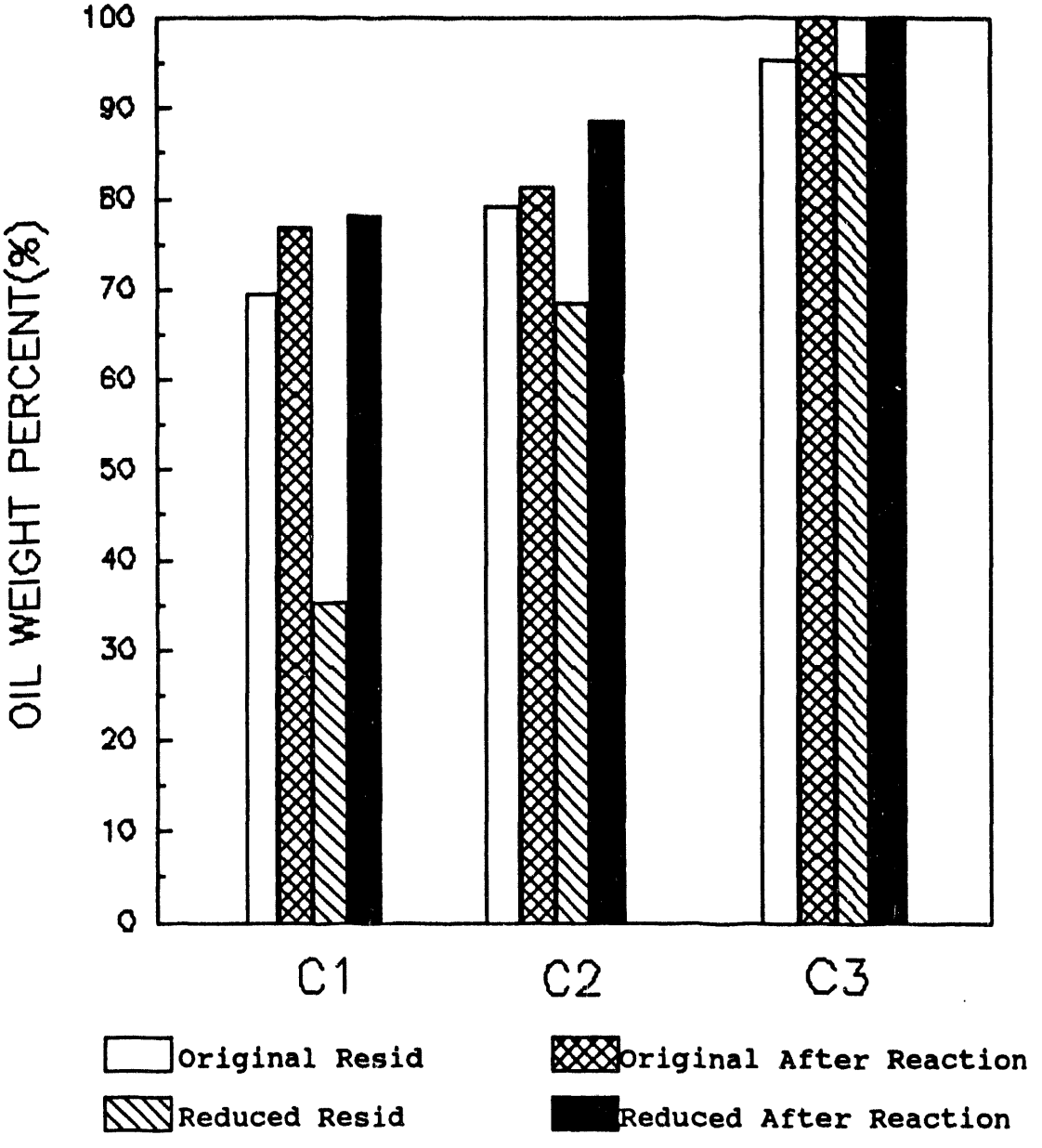
* (−) mean mole hydrogen released was larger than mole hydrogen used.

ISO = isotetralin
ANT = anthracene
TET = tetralin
PHP = perhydropyrene
PYR = pyrene
HHA = hexahydropyrene
DHA = dihydropyrene
PHA = perhydroanthracene



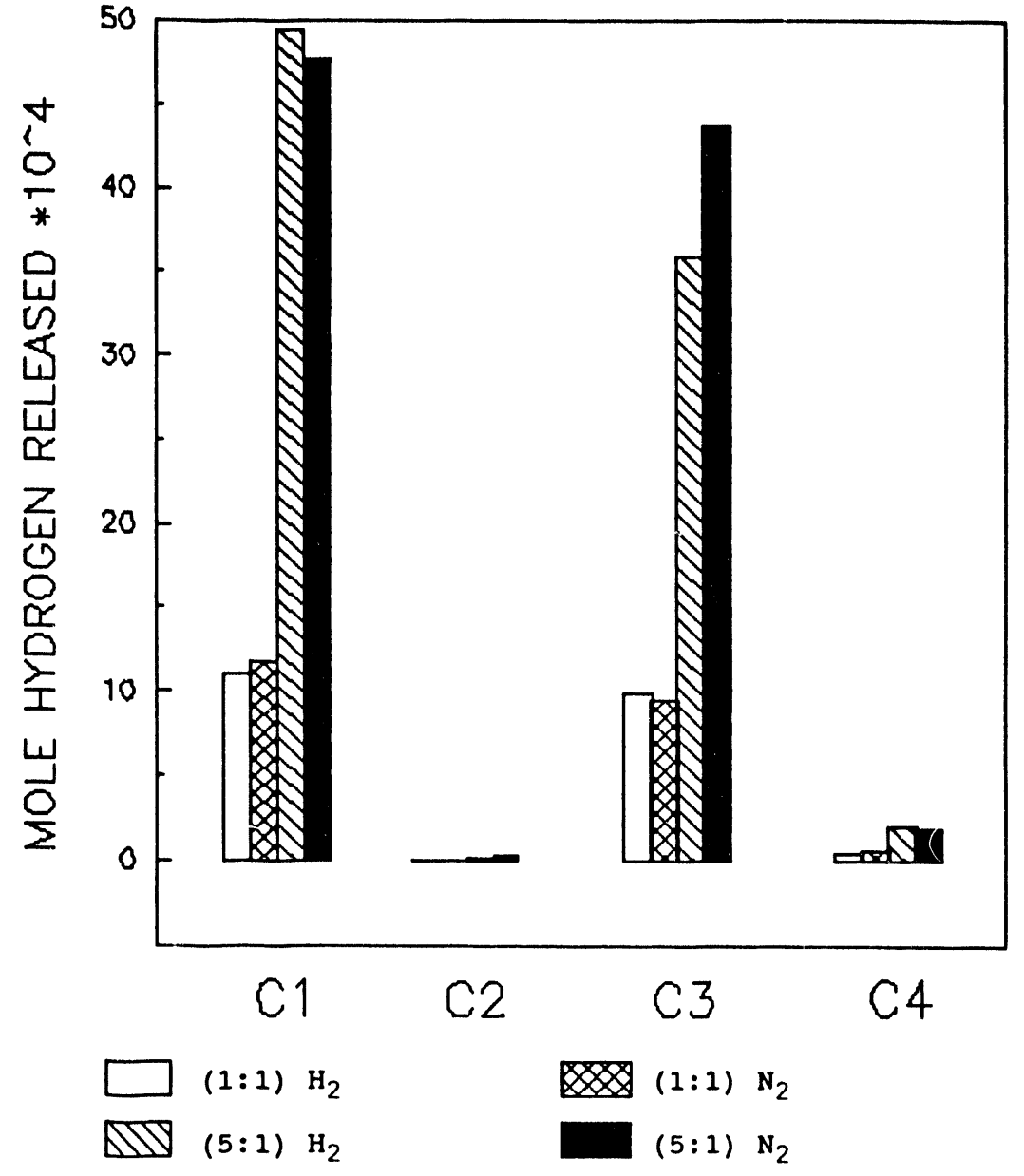
C1= MAYA
C2= DAU
C3= S.LA.

Figure 1. Comparison of the Oil Fractions of the Original and Reduced Resids Before and After Reactions with Anthracene and Perhydropyrene in Nitrogen



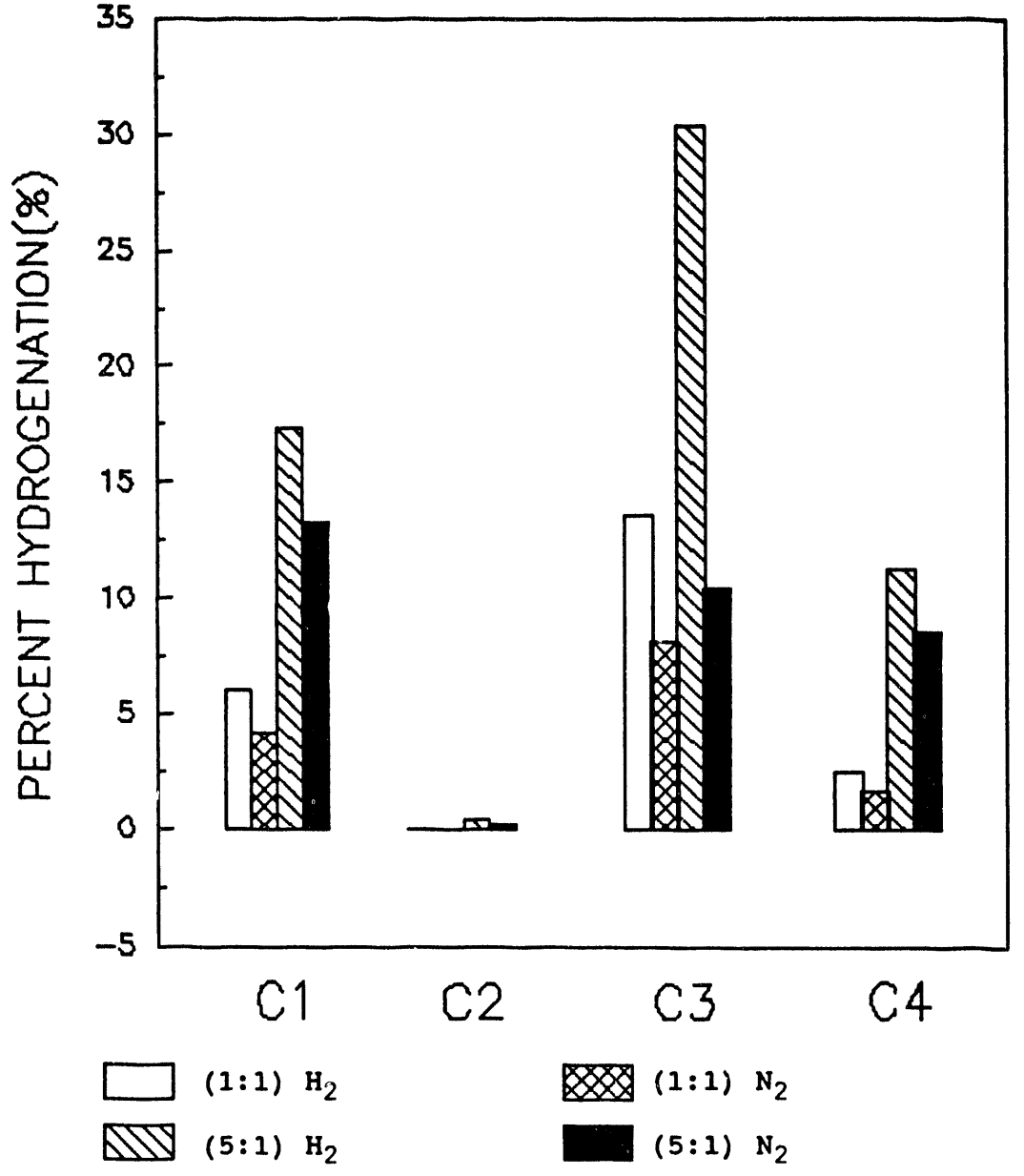
C1= MAYA
C2= DAU
C3= S.LA.

Figure 2. Comparison of the Oil Fractions of the Original and Reduced Resids Before and After Reactions with Anthracene and Perhydropyrene in Hydrogen



C1= ISO/PYR thermal
C2= TET/PYR thermal
C3= HHA/PYR thermal
C4= DHA/PYR thermal

Figure 3. Hydrogen Released by Hydrogen-Rich Species for Reactions of Hydrogen-Rich Species with Pyrene.



C1= ISO/PYR thermal
C2= TET/PYR thermal
C3= HHA/PYR thermal
C4= DHA/PYR thermal

Figure 4. Percent Hydrogenation of Aromatics Obtained in Reactions with Hydrogen-Rich Species.

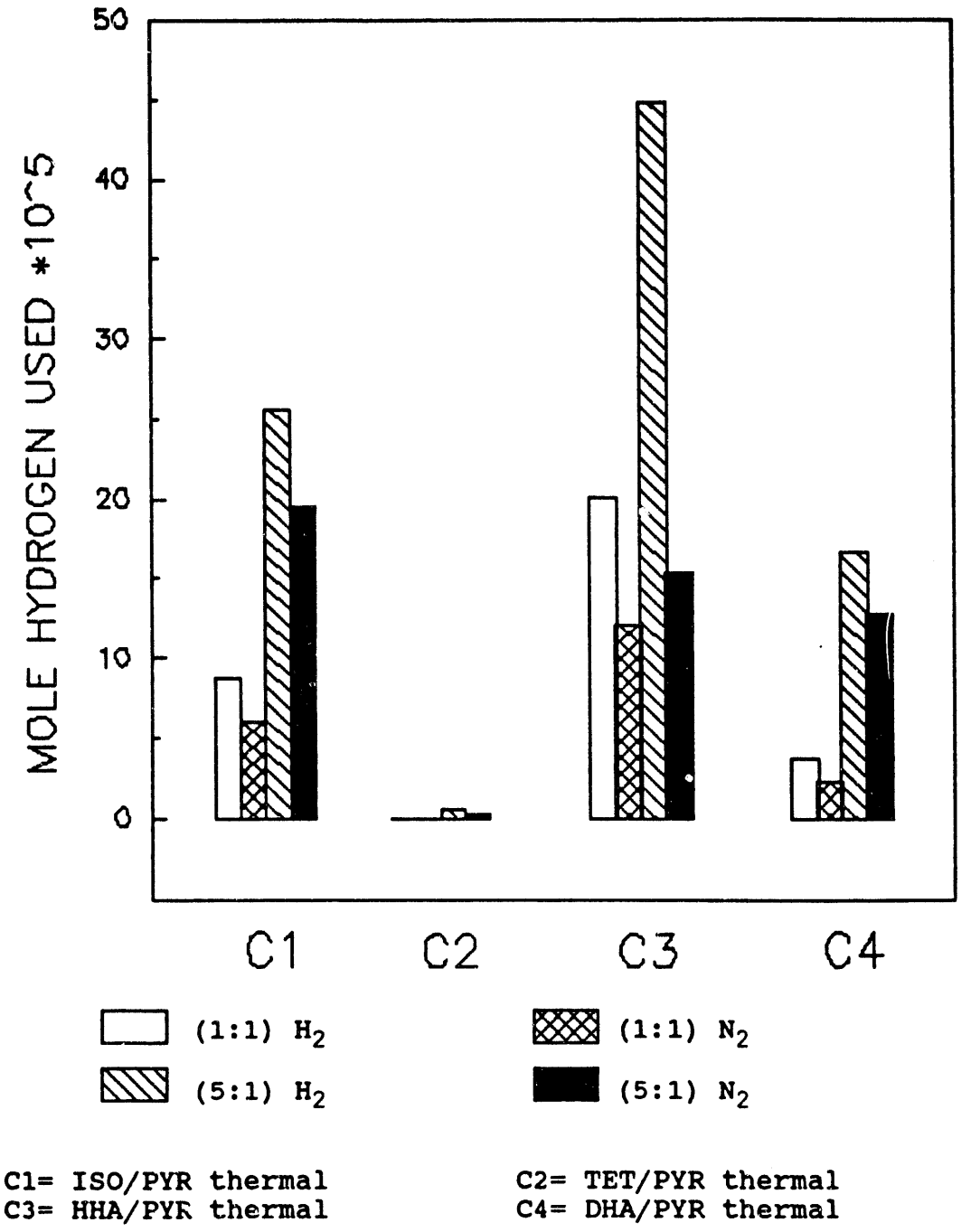
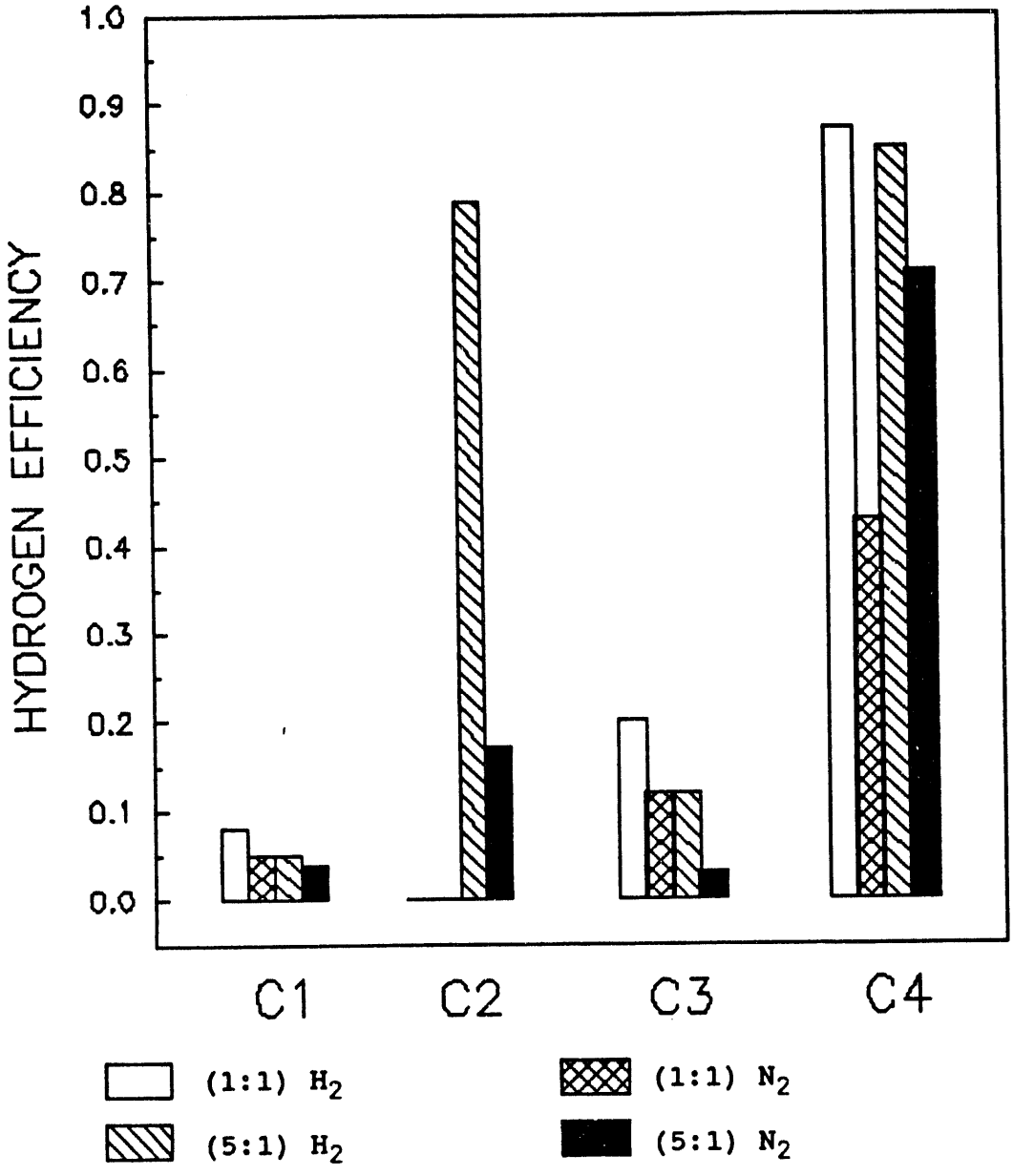
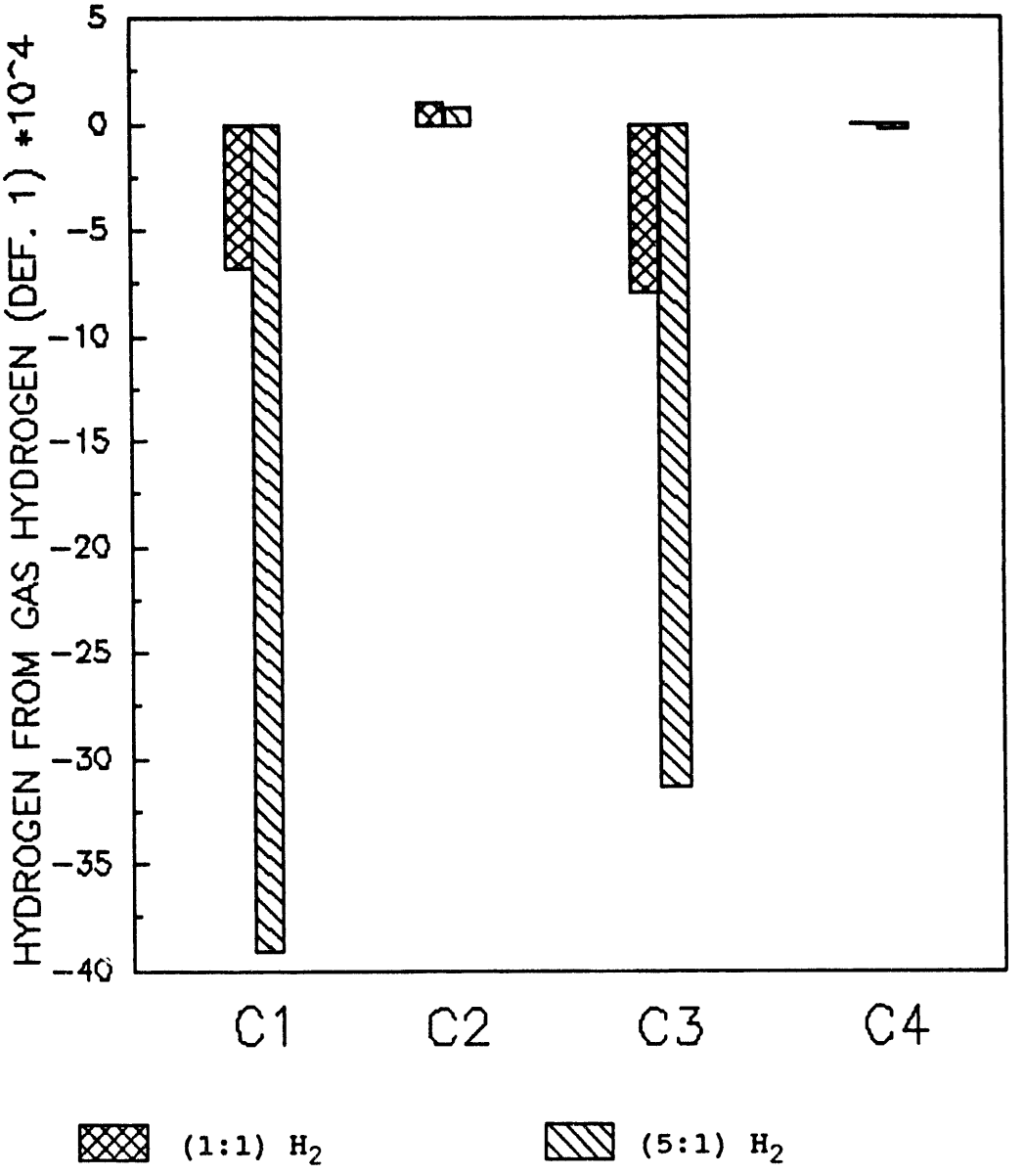


Figure 5. Hydrogen Used by Pyrene for Reactions of Hydrogen-Rich Species with Pyrene.



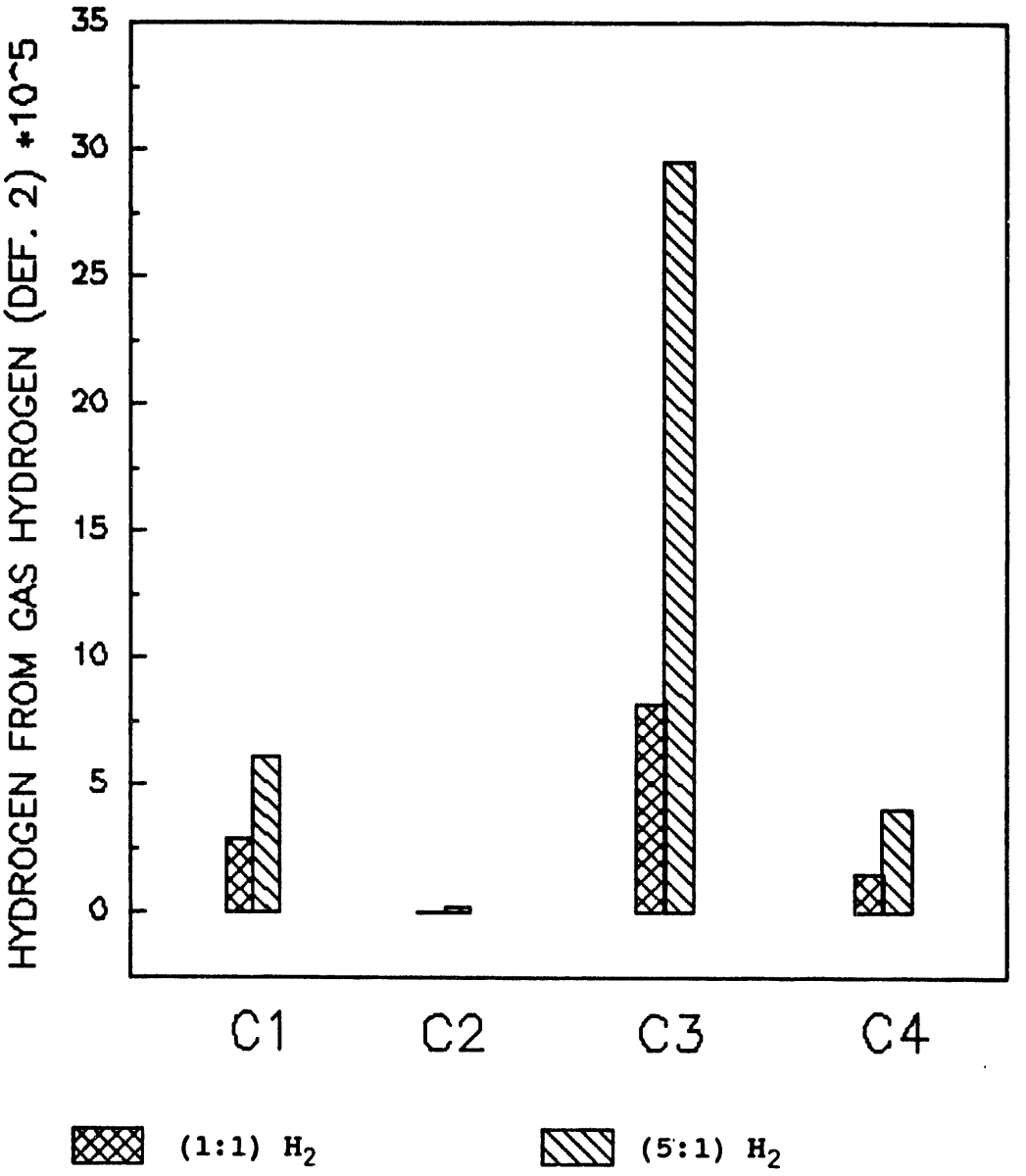
C1= ISO/PYR thermal
C2= TET/PYR thermal
C3= HHA/PYR thermal
C4= DHA/PYR thermal

Figure 6. Hydrogen Efficiency for Reactions of Hydrogen-Rich Species with Pyrene.



C1= ISO/PYR thermal
C2= TET/PYR thermal
C3= HHA/PYR thermal
C4= DHA/PYR thermal

Figure 7. Moles of Hydrogen which Came from Gas Hydrogen for Reactions of Hydrogen-Rich Species with Pyrene. (Definition 1)



C1= ISO/PYR thermal
C2= TET/PYR thermal
C3= HHA/PYR thermal
C4= DHA/PYR thermal

Figure 8 . Moles of Hydrogen which Came from Gas Hydrogen for Reactions of Hydrogen-Rich Species with Pyrene. (Definition 2)

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