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DETERMINATION OF H-DONOR ABILITY OF HEAVY OILS/BITUMENS AND ITS IMPORTANCE IN COPROCESSING

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OBJECTIVES

* TO DETERMINE WHETHER HEAVY OILS AND BITUMENS ARE HYDROGEN DONORS

* TO INVESTIGATE THE ROLE OF HEAVY OILS AS HYDROGEN DONORS IN COPROCESSING

BEHAVIOR OF "SOLVENT" UNDER COAL LIQUEFACTION AND COPROCESSING

* IN COPROCESSING THE SOLVENTS ARE ALSO REACTANTS

* IN COPROCESSING FRESH SOLVENT IS SUPPLIED CONTINUOUSLY TO THE SYSTEM

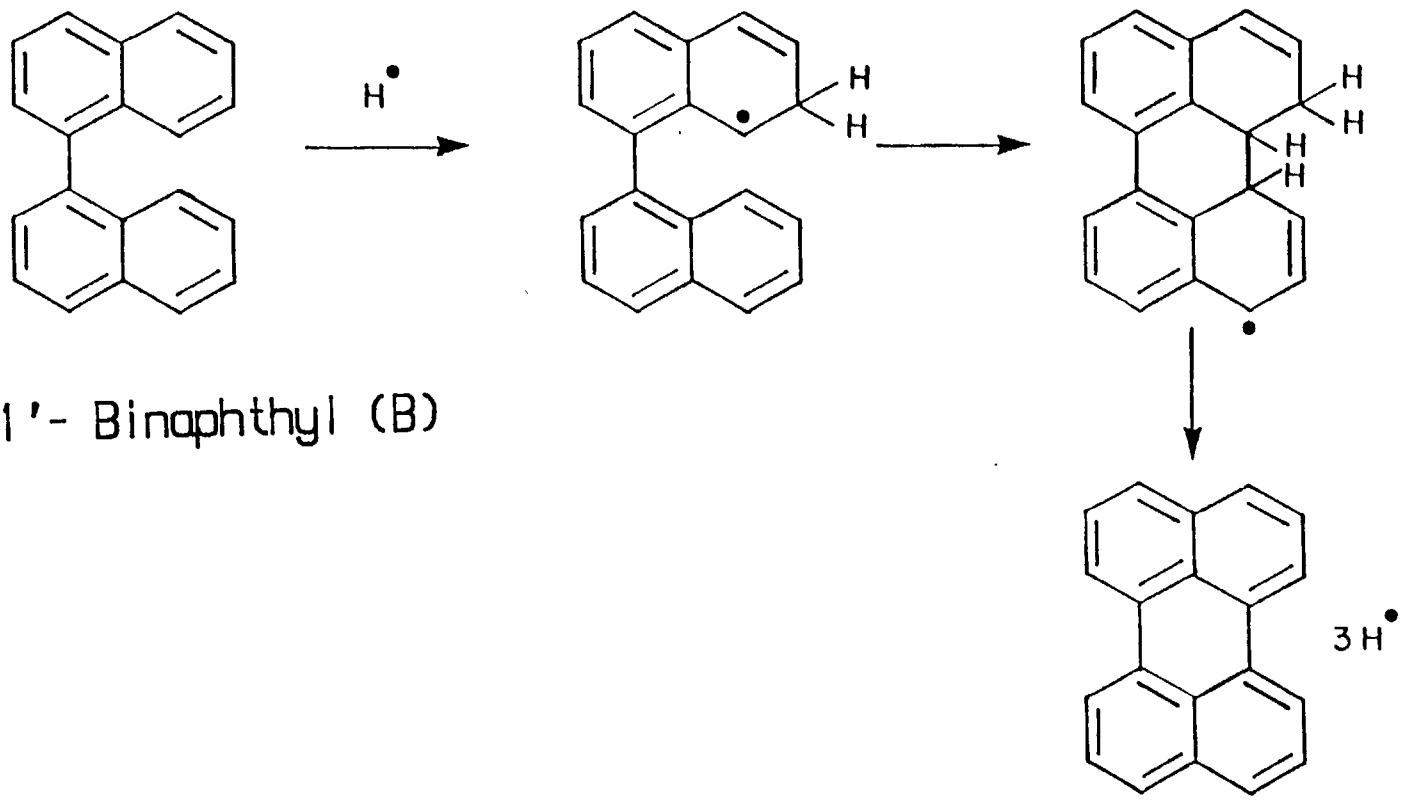
* UNLIKE LIQUEFACTION, THE QUALITY OF COPROCESSING SOLVENT IS MAINTAINED DURING THE PROCESS

H-DONOR ABILITY MEASUREMENTS

* 1,1'-BINAPHTHYL $\xrightarrow[430\ ^{o}C]{\text{H-DONOR}}$ PERYLENE

* SULPHUR $\xrightarrow[235\ ^{o}C]{\text{H-DONOR}}$ H_2S

* ^{13}C NMR



1,1'- Binaphthyl (B)

perylene (P)

Analysis of Forestburg coal

Proximate analysis
(wt %, as received)

Moisture	14.09
Volatile matter	36.37
Fixed carbon	42.67
Ash	6.87

Ultimate analysis
(wt % daf)

C	71.99
H	4.64
N	1.78
O	20.98
S	0.61

Elemental Analyses of Oil Feedstocks (wt %)

Solvents/Oils	C	H	N	O	S
CLVB[a]	82.82	10.57	0.78	0.35	5.66
CLVB(P)[b]	82.62	10.27	0.83	0.26	5.79
Boscan	80.96	10.24	0.90	0.24	5.73
Boscan(P)[b]	81.97	9.83	1.09	0.29	6.40
Maya	84.80	10.10	0.42	< 0.50	4.30
Blend 24[c]	84.31	10.90	0.81	0.33	3.45
Athabasca	82.30	9.60	0.67	0.69	5.96
IPPL[d]	86.40	10.90	0.43	< 0.50	1.71
Lloydminster	83.20	9.84	0.54	0.61	5.73
Raw anthracene oil	91.50	5.74	1.04	0.56	0.58
Hydrogenated anthracene oil	90.60	9.10	0.15	0.26	0.00

[a] Cold Lake vacuum bottoms, [b] +525°C fractions, [c] Venezuela blend,
[d] blend of Western Canadian crudes (IBP = 560°C)

Characteristics of Oil Feedstocks (heavy oils/bitumens)

Solvents/ Oils	Pentane Inso.(wt %)	Toluene Inso.(wt %)	Pitch[a] wt %	CCR wt %	gravity (°API)	Mn[1]	f_a[2]
CLVB[b]	23.5	0.20	83.2	17.1	4.82	788	31
Boscan	22.3	0.09	64.6	16.7	7.77	613	30
Maya	22.3	0.11	86.0	18.4	----	756	34
Blend 24[c]	21.5	<0.10	95.1	18.6	6.95	848	30
Athabasca	38.4	1.21	99.3	23.9	1.49	983	34
IPPL[d]	14.0	0.92	100.0	15.6	9.86	910	30
Lloydminster	37.4	0.22	90.7	22.0	3.39	1081	35

[a] +525°C fraction, [b] Cold Lake vacuum bottoms, [c] Venezuela blend, [d] blend of Western Canadian crudes (IBP=560°C), [1] number average molecular weight (VPO), [2] aromaticity (^{13}C NMR)

EXPERIMENTAL CONDITIONS FOR COPROCESSING

REACTOR	100 mL SHAKING AUTOCLAVE
COAL TYPE	FORESTBURG SUBBITUMINOUS
COAL CONCENTRATION	30 WT. % MAF
CATALYST	IRON SULPHATE
TEMPERATURE	420 °C
PRESSURE	5.52 MPA H_2 COLD
RESIDENCE TIME	30 MIN. AND 5 MIN.

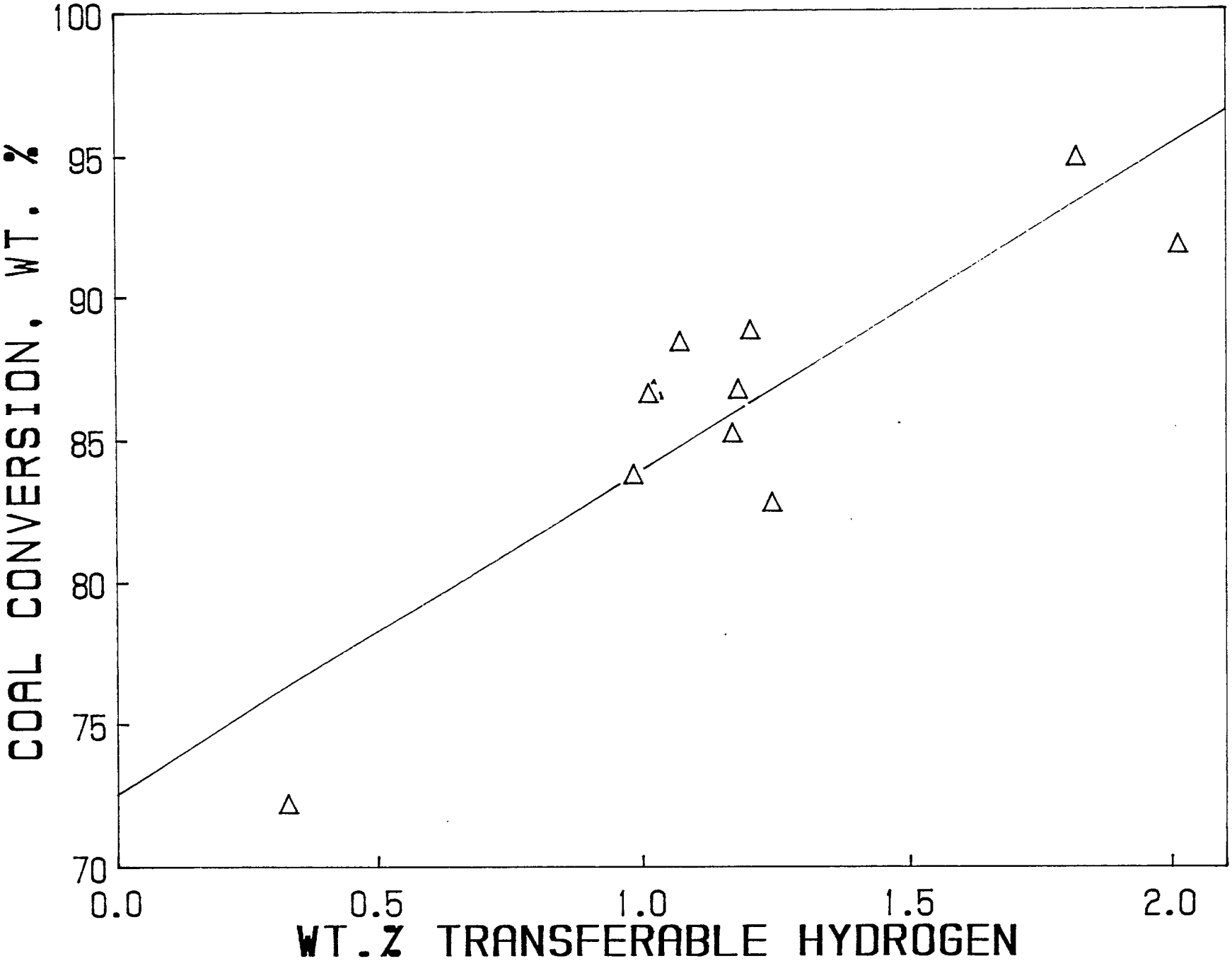
H-donor ability of heavy oils/bitumens using 1,1'-binaphthyl

Material	P/B X 100	Coal Conversion (WT. %)	
		H_2 .30 min.	N_2 .5 min
1,1'-Binaphthyl	0.19	----	----
Tetralin	0.51 ± 0.03	91.7	59.8
9,10-DHA	10.0 ± 1.5	----	----
CLVB	5.5 ± 0.6	88.7	22.1
CLVB(P)	6.9 ± 0.3	----	----
Boscan	5.4 ± 0.4	88.3	20.1
Boscan(P)	7.2 ± 0.2	85.1	21.3
Maya	7.0 ± 1.1	82.7	19.1
Blend 24	5.7 ± 0.6	86.7	21.9

comparison of H-donor abilities and coal conversions

Solvent	Transferable Hydrogen (wt. %)		Coal Conversion (wt. %)	
	Sulphur	^{13}C nmr	H_2 .30 min.	N_2 .5 min
Tetralin	2.01	----	91.7	59.8
CLVB	1.20	1.28	88.7	22.1
Blend 24	1.01	1.32	86.5	21.9
Athabasca	1.02	1.30	86.6	20.8
Maya	1.07	1.13	82.7	19.1
Boscan	1.24	----	88.3	20.1
Boscan(P)	1.17	----	85.1	21.3
IPPL	0.98	----	83.7	19.1
Lloyd.	1.18	----	86.6	20.0
RAO	0.33	----	72.1	26.1
HAO	1.82	----	94.8	78.2

COAL CONVERSION AS A FUNCTION OF DONATABLE HYDROGEN



Hydrocarbon type separation of heavy oils/bitumens (wtZ)

Solvent	Saturates	Aromatics	Polars
CLVB	28.66	58.68	12.66
Blend 24	36.38	51.13	12.49
Athabasca	19.5	65.81	14.68
Maya	41.51	50.82	7.68

CONCLUSIONS

* ALTHOUGH LIMITED AMOUNTS OF TRANSFERABLE HYDROGENS ARE PRESENT IN HEAVY OILS/BITUMENS, HIGH COAL CONVERSIONS ARE USUALLY OBTAINED

* GOOD CORRELATION (USING SULPHUR AS HYDROGEN ACCEPTOR) WAS OBTAINED BETWEEN COAL DISSOLUTION IN HEAVY OILS/BITUMENS AND H-DONOR ABILITY

CONCLUSIONS

* IN COPROCESSING, COAL DISSOLUTION IS NOT AFFECTED BY THE CONCENTRATION OF SATURATES AND ASPHALTENES FRACTIONS

* IN TERMS OF COAL DISOLUTION AND UNDER THE PROCESS CONDITIONS EMPLOYED THERE IS LITTLE DIFFERENCE BETWEEN BITUMENS AND CONVENTIONAL RESIDS