

**GEOCHEMICAL STUDIES - 3
GEOCHEMISTRY OF SOME
ALBERTA SHALES AND
ASSOCIATED KEROGEN**

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"GEOCHEMICAL STUDIES"

This series of reports, under the general title "Geochemical Studies", makes available geochemical data on the formation fluids and rocks of Alberta which would otherwise remain unpublished. Two types of data fall in this category. First, "Geochemical Studies" will act effectively as a document depository in cases where a formal publication is available, but without the raw data having been published; additional interpretations may be included if pertinent. Second, "Geochemical Studies" will include both the raw data and a minimal descriptive report in the case where no formal publication is planned.

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ABSTRACT

A set of 28 shales from the Alberta Basin, ranging in age from Late Cretaceous to Middle Cambrian, was studied with respect to their major and trace element composition, and the kerogen extracted from 25 of them for detailed analysis. This Open File report contains the basic data on the shales and kerogen. It is not intended to report this information elsewhere.

Although the shales are widely scattered areally, on a volumetric basis the Upper Cretaceous is underrepresented and the Lower Cretaceous overrepresented. The average for 24 non-calcareous shales from the Alberta Basin is close to the average shale in geosynclines. A decrease in SiO_2 content with age suggests a decrease in silt (quartz) content rather than a change in clay mineralogy. General statistics are provided for groups of shales based on the three crude oil families distinguished by previous authors i.e. Group 1: U. Cretaceous Colorado and post-Colorado reservoirs; Group 2: L. Cretaceous Mannville Group, Jurassic, Carboniferous and U. Devonian Wabamun Group reservoirs; Group 3: U. Devonian Winterburn and Woodbend Groups and Beaverhill Lake Formation reservoirs. For Cd, Cr, Mn, Fe, Co, Ni and Mo there is no significant difference among the three groups of shales. Sodium in formation water and crude oil increases with depth, whereas, for reasons not clear, Na in shales decreases. The sharp decrease in the contents of Zn, Cu and Pb with depth is associated with the increased salinity (chloride content) of the associated formation waters and may relate to the greater ease of removal of these elements from shales as chloride complexes of the metals.

The majority of the kerogen samples are Type III, the rest being Type II; with one exception they are low-S types. Using estimated maximum temperature from a previous study, it is suggested that there is a tendency for loss of both O and S with increased temperature and therefore a relative increase in N as a residual effect. With respect to the ESR properties of the kerogen, increased temperature results in increased spin concentrations, lower g-values, and wider lines. At any specific temperature, there is a wide range in the NMR aliphatic-carbon/aromatic-carbon ratio.

INTRODUCTION

The Alberta Basin is well explored, with abundant geological and geochemical data. Comprehensive reports are available on the geochemistry of crude oils and of hydrocarbons extracted from potential source rocks, but there is only one published study (McIver, 1967) on the geochemistry of kerogen extracted from shales. Accordingly, a suite of 28 shales was collected in the late 1970s from several sources, in an attempt to represent major argillaceous units both stratigraphically and areally (Figure 1). However, when the relative volumes of shales in the main stratigraphic units are compared with the proportion of samples from the same unit (Table 1) the Upper Cretaceous is underrepresented and the Lower Cretaceous overrepresented. Most of the samples are from core stored by the Alberta Energy Resources Conservation Board; two samples (RCA 65-1, RCA 67-1) are from core from shallow test holes drilled by the Alberta Research Council.

The purpose of this Open File report is to present (Appendix A) details of the stratigraphy, location, depth, sample description and depositional environment (determined from geological information) of these 28 samples, together with inorganic and organic determinations. Properties of the associated kerogen are included if the kerogen was extracted. There is a brief description of the analytical techniques but minimal interpretation of the data. This Open File report contains the only summary of the geochemistry of these shales and their associated kerogen.

ANALYTICAL PROCEDURES

SHALES

Samples were chipped clean and crushed in a shatterbox to pass 325 mesh. The partial major element analysis carried out by Barringer Research Limited (Rexdale, Ontario) has been converted to oxide percentages in the data tables in Appendix A. Twelve trace elements (Ag, Cd, Co, Cr, Cu, Mn, Mo, Ni, Pb, Sr, V, Zn) were also determined by Barringer Research Limited using a multielement radio frequency emission spectrometer following lithium metaborate fusion. Detection limits (ppm) are as follows: Ag 0.004; Cd 0.002; Co 0.003; Cr 0.001; Cu 0.001; Mn 0.001; Mo 0.005; Ni 0.006; Pb 0.008; Sr 0.00002; V 0.006; Zn 0.002 (these detection limits refer to pure solutions).

Organic C and extractable organics were determined by the Institute of Sedimentary and Petroleum Geology, Geological Survey of Canada (Calgary, Alberta). Vitrinite reflectance and organic matter petrography determinations (Appendix B) were carried out on selected samples by Institut Nationale de la Recherche Scientifique, Universite du Quebec (Ste. Foy, Quebec).

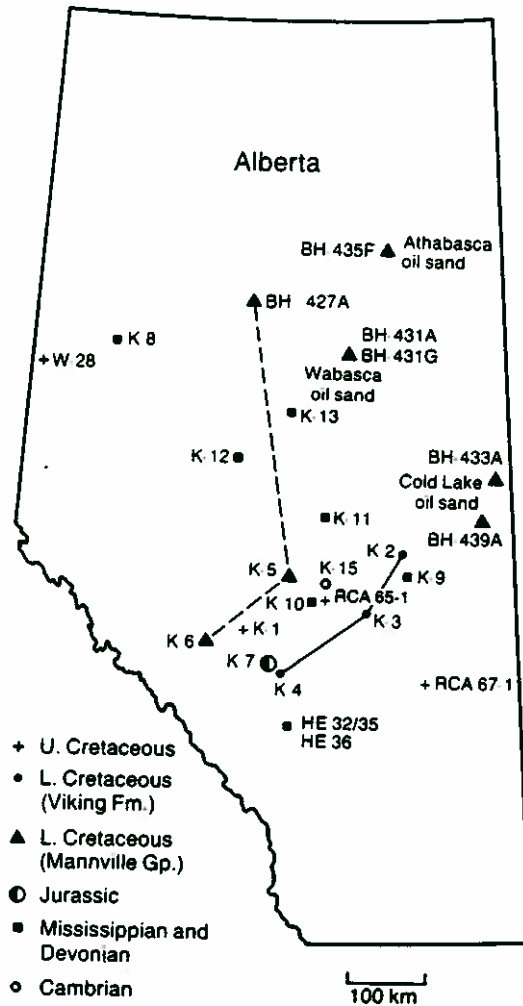


Figure 1. Distribution of Alberta shales studied. Solid tie line joins samples from the Viking Formation, and dashed tie line joins samples from the non-oilsands Mannville Group.

Table 1. Comparison of the proportions of shale and shale-samples in selected stratigraphic units. Alberta Basin shale volumetric data from Hitchon (1968).

Stratigraphic Unit	Shale			Samples studied	
	% Total basin	% in unit	% Total shale in basin	No.	% Total
Tertiary	1.3	75.0	1.8	-	-
U. Cretaceous	27.3	92.6	44.3	4	14
L. Cretaceous	13.8	73.1	17.8	11	39
Jurassic	2.4	57.7	2.4	1	3.5
Triassic	2.0	75.7	2.6	-	-
Permian	0.4	15.3	0.1	-	-
Carboniferous	9.0	35.5	5.6	3	11
U. Devonian	22.0	36.4	14.1	5	18
M. Devonian	9.0	15.7	2.5	3	11
Silurian	1.3	5.0	0.1	-	-
Ordovician	3.3	15.0	0.9	-	-
Cambrian	8.2	54.1	7.8	1	3.5

KEROGEN

Kerogen was separated using the techniques described by Hitchon et al. (1976), in which digestions were held at 40°C and took place under N₂ to avoid an increase in the number of free radicals in the kerogen as a result of conventional hot HF digestion. After digestion in 2N HCl, the residue was centrifuged and washed with hot water until free of Ca ions. Following digestion with 48% HF, a few millilitres of 2N HCl were added to the solution, which was then diluted with a saturated boric acid solution, centrifuged, and washed with hot water. The residue was then centrifuged in a mixture of bromoform and acetone (6:1) to separate the kerogen from pyrite. X-ray diffraction showed K-fluossilicate in all kerogen samples, which was entirely removed with copious volumes of hot water. Only three samples (RCA 65-1, K-1, BH-439A) contained significant amounts of ralstonite, which was quantitatively extracted with 6N HCl at 70°C and analyzed (Hitchon et al., 1976).

Elemental composition was determined by Alfred Bernardt Mikroanalytisches Laboratorium (Elbach uber Engelskirchen, Germany), with O determined directly. The elemental composition in Appendix A is normalized (Sum CHONS=100) and adjusted for pyrite-S (%Fe x 1.1482). Although it was difficult to remove the entrained pyrite

completely (Fe 1 to 22%, mean 8.5%) clean-up of the pyrite separates for S isotope determination was relatively successful; C in 13 pyrite concentrates was in the range 1.3 to 11.8% (average 4.9%).

The ESR properties were determined by Dr. K.F. Schulz, Alberta Research Council on a Varian Model 4500 ESR spectrometer, operating at a nominal frequency of 9.3 GHz, with power levels maintained low enough to avoid saturation effects. Although samples were run in air and *in vacuo* only the latter results are reported here. Corrections were made for the pyrite content (range 1.97-47.47%; average 18.5%). A check on the technique used was made by analysing kerogen previously analysed by the Institut Francais du Petrole (B. Durand, personal communication); Table 2 shows that the results are in close agreement.

The solid state ^{13}C NMR spectra were obtained at 22.6 MHz on a Bruker CXP180/90 NMR spectrometer using the cross polarization (CP) technique with magic angle spinning (MAS). A contact time of 1 ms and a repetition time of 2 s were selected. The MAS speeds were 3-3.4 KHz. Chemical shifts were determined by substitution relative to tetramethylsilane (TMS). Each spectrum was the Fourier transform of 3000-10,000 free-induction decay curves. The ^{13}C NMR spectra were run by Dr. John Ripmeester (Division of Chemistry, National Research Council of Canada, Ottawa, Ontario).

Sulfur isotopes were determined by Professor H.R. Krouse (The University of Calgary) on the kerogen, pyrite and extractable organic matter on selected samples, depending on sample size available.

GEOCHEMISTRY OF ALBERTA SHALES

AVERAGE BULK COMPOSITION

The average of 24 non-calcareous shales from Appendix A is close to that for the average shale in geosynclines (Table 3). The four samples not included in Table 3 had either anomalous total oxides (RL 2/4, K-16) or were calcareous (HE 32/35, K-12) with indeterminate CaO content (>9.2%). Individual major oxides, however, show wide concentration ranges (see Table 3). In part, these wide concentration ranges are a reflection of the wide ranges of depositional environments, diagenesis and hence mineralogy of shales in the Alberta Basin. For example, many analyses reporting $\text{SiO}_2 > 60\%$ are from shales classified as 'silty', although it is recognized that this classification is highly subjective without a grain size analysis. The highest SiO_2 (77%, RCA 67-1) is from a shale reported as

Table 2. Comparison of ESR parameters on kerogen separated from Toarcian shales, Paris Basin.

		Alberta Research Council	Institut Francais du Petrole
Ancerville	Spin No. ($\times 10^{18}$)	1.2	-
	g-value	2.00285	-
	Line width (mT)	5.7	-
Bouchy	Spin No. ($\times 10^{18}$)	4.1	4.7
	g-value	2.00287	2.0028
	Line width (mT)	6.3	6.4
Essises	Spin No. ($\times 10^{18}$)	1.4	2.5
	g-value	2.00278	2.0029
	Line width (mT)	6.1	6.1
Cesarville	Spin No. ($\times 10^{18}$)	1.2	1.9
	g-value	2.00274	-
	Line width (mT)	7.2	5.1
Vacherauville	Spin No. ($\times 10^{17}$)	3.8	5.2
	g-value	2.00300	-
	Line width (mT)	6.0	5.7
Joinville	Spin No. ($\times 10^{17}$)	5.6	6.2
	g-value	2.00269	-
	Line width (mT)	8.3	6.7
Dontrien	Spin No. ($\times 10^{17}$)	0.7	1.2
	g-value	2.00281	-
	Line width (mT)	8.2	5.6

Table 3. Comparison of the composition (%) of non-calcareous Alberta Basin shales with average geosynclinal and platform shales (from Wedepohl, 1969, Table 8-4).

	Alberta Basin (n=24)*		Shales (geosynclines) (n=277)	Shales (platforms) (n=6800)
	Average	Range		
SiO ₂	58.4	32-77	58.9	50.7
TiO ₂	0.6	0.3-0.9	0.78	0.78
Al ₂ O ₃	14.8	9-26	16.7	15.1
Fe as Fe ₂ O ₃	5.1	2.9-11.6	6.9	6.7
MnO	0.04	0.01-0.12	0.09	0.08
MgO	2.0	0.8-4.7	2.6	3.3
CaO	1.4	0.2-9.1	2.2	7.2
Na ₂ O	0.3	0.0-0.7	1.6	0.8
K ₂ O	-	-	3.6	3.5
H ₂ O+	-	-	5.0	5.0
P ₂ O ₅	-	-	0.16	0.10

*Data from Appendix A, except RL 2/4, HE 32/35. K-12 and K-16.

'bentonitic'. Although there are only a few data, there is a suggestion that the SiO₂ content of non-calcareous shales in the Alberta Basin decreases with age e.g.

	No.	Avg. SiO ₂	Avg. Al ₂ O ₃
U. Cretaceous	4	67	14.8
L. Cretaceous (L. Colorado Gp.)	3	65	13.7
L. Cretaceous (Mannville Gp.)	8	57	15.6
Mississippian and Devonian	8	52	14.0

This trend is not reflected in the Al₂O₃ content and might relate to a decrease in silt (quartz) content, rather than a change in clay mineral content.

Other particularly high contents of individual major oxides include 11.6% Fe₂O₃ and 0.12% MnO in sample BH-427A, which contained pyrite nodules. The range for TiO₂ and Na₂O is quite narrow.

TRACE ELEMENT GEOCHEMISTRY

Introduction

Based on a very comprehensive study, Deroo et al. (1977) distinguished three crude oil families in Alberta, as follows:

Group 1	U. Cretaceous Colorado and post-Colorado reservoirs
Group 2	L. Cretaceous Mannville Group, Jurassic, Carboniferous and U. Devonian Wabamun Group reservoirs
Group 3	U. Devonian Winterburn and Woodbend Groups and Beaverhill Lake Formation reservoirs

Hitchon and Filby (1983) used simple statistics and an ANOVA, and subsequently the same authors used stepwise multiple-discriminant function analysis and multiresponse permutation procedures (Hitchon and Filby, 1984) to show that trace elements can also be used to classify crude oils into families. All these studies dealt with either the organic (Deroo et al., 1977) or inorganic (Hitchon and Filby, 1983, 1984) parts of crude oils. However, crude oils originate from source rocks, dominantly shales, and there could well be geochemical links between the trace elements in source rocks, those in associated crude oils, and indeed in the associated formation water, the carrier medium for hydrocarbon migration. Hitchon and Filby (1983) pointed out some of these possible links and indicated where future research might be directed. With this latter objective in mind the following notes are intended to point out some interesting simple statistical trends which may have some veracity. However, extreme caution must be used in any extrapolation from such small and varied populations. As appropriate, the data bases used were Appendix A (this report) for shales, Hitchon and Filby (1983) for crude oils and Hitchon et al. (1971) for formation waters. The three groups for each data set were as determined by Deroo et al. (1977).

Alkali Metals - Sodium

General Statistics

Na (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	7	900	3800	3400	5400
Crude oils (n=20)	20	0.046	0.73	1.54	13.0
Formation waters (n=15)	15	1510	7260	8080	22800
GROUP 2					
Shales (n=12)	12	200	1400	2000	5100
Crude oils (n=25)	22	0.018	0.83	2.94	19.3
Formation waters (n=25)	25	510	10600	15200	42900
GROUP 3					
Shales (n=7)	7	300	900	1300	3500
Crude oils (n=33)	33	0.0174	0.632	4.61	64.7
Formation waters (n=34)	34	9360	48900	48100	92800

Geochemistry

Although Na, Rb and Cs were determined in the crude oils, and Na, K and Rb in the formation waters, only Na was determined in the shales. The average depths are 950 m, 1270 m and 1960 m for shales from groups 1 to 3, respectively, so the marked increase in the median, average and maximum contents of Na in the formation waters is to be expected given the general increase of salinity with depth. There is a similar trend for the average and maximum contents of Na in the crude oils; this is not, however, a result of entrained formation water (see discussion in Hitchon et al., 1975) but likely related to pH effects and the fact that Na in crude oil probably occurs as the Na salt of a petroleum acid (see discussion in Hitchon and Filby, 1983, pp. 14-16). What is most interesting in the general statistical data is the decrease in the minimum, median, average and maximum for Na in shales, opposite to the trends in the two fluids. At this time there is no obvious explanation.

Alkaline Earth Metals - Magnesium, Calcium and Strontium

General Statistics

Mg, Ca, Sr (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	Mg 7	7000	9400	9700	12200
	Ca 7	2000	2700	3900	8300
	Sr 7	62	170	135	183
Formation waters (n=15)	Mg 13	8	46	95	409
	Ca 15	14	72	211	1230
	Sr 15	0.52	20	40	219
GROUP 2					
Shales (n=12)	Mg 12	4500	12300	12600	28300
	Ca 11	1500	4100	9900	31700
	Sr 12	46	160	177	352
Formation waters (n=25)	Mg 25	2	68	370	1760
	Ca 25	12	223	1400	9740
	Sr 25	0.27	26	123	539
GROUP 3					
Shales (n=7)	Mg 7	4400	14100	12400	19800
	Ca 6	16000	22800	28600	65000
	Sr 7	10	182	227	658*
Formation waters (n=34)	Mg 34	428	2230	2320	3990
	Ca 34	1380	17700	17000	38700
	Sr 34	36	644	624	1320

*without this extreme value ($>3\sigma$ from the mean for all shales) the median, average and maximum values are 172, 156 and 279 ppm, respectively.

Geochemistry

For the alkaline earth metals, data are available only for shales and formation waters. In the formation waters, there is a general increase in all alkaline earths with depth, and the order is uniformly $\text{Ca} > \text{Mg} > \text{Sr}$. In the shales the order is generally $\text{Mg} > \text{Ca} > \text{Sr}$ for groups 1 and 2, but is $\text{Ca} > \text{Mg} > \text{Sr}$ for group 3, almost certainly due to the presence of calcite in the shales. A ternary diagram (Figure 2) of average values for $[\text{Ca}+\text{Mg}+\text{Sr} \times 10=100]$ shows that both shales and formation waters have a marked

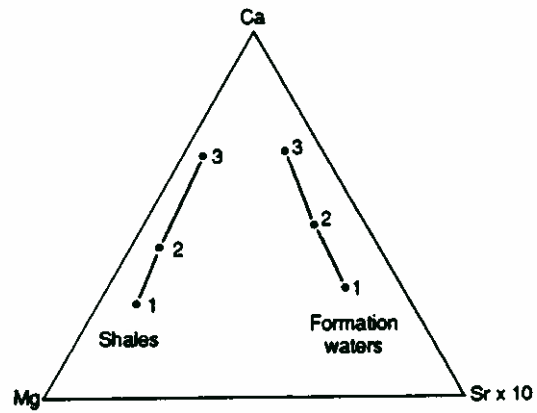


Figure 2. Relations of average values of $[Ca+Mg+Srx10=100]$ in shales and formation waters from 3 groups.

increase in Ca with depth going from group 1 to group 3, mainly at the relative expense of Mg in the case of shales and Sr in the case of formation waters. It is suggested that the effect in shales results essentially from the presence of calcite in increasingly calcareous rocks going from group 1 to group 3 (see trends in Hitchon, 1968, Figures 3 and 4). The trend in the formation waters possibly relates to solubility effects. In a recent study of formation waters from northern Alberta, Hitchon (1993) showed that the control on the content of Sr is by means of different Sr-minerals, depending on the hydrostratigraphic unit -- or more precisely, on parameters such as SO₄ content and dissolved CO₂ species, which generally vary with depth.

Zinc and Cadmium

General Statistics

Zn, Cd (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	Zn 7	99	161	270	943*
	Cd 7	6.4	13	15	26
Crude oils (n=20)	Zn 20	0.0115	0.270	0.272	0.670
Formation waters (n=15)	Zn 15	0.00	0.08	0.36	3.05
	Chloride 15	798	-	12200	38200
GROUP 2					
Shales (n=12)	Zn 12	65	126	132	261
	Cd 12	10	13	14	22
Crude oils (n=25)	Zn 24	0.0175	0.401	0.456	1.277
Formation waters (n=25)	Zn 25	0.03	0.13	0.32	3.05
	Chloride 25	320	-	25700	95800
GROUP 3					
Shales (n=7)	Zn 7	19	60	61	100
	Cd 7	1.1	14	9	16
Crude oils (n=33)	Zn 28	0.0134	0.140	0.573	5.921
Formation waters (n=34)	Zn 34	0.05	0.16	1.43	27.5
	Chloride 34	15800	-	69700	172000

*without this extreme value (>3σ from the mean for all shales), the median, average and maximum values are 158, 158 and 206 ppm, respectively.

Geochemistry

Hitchon (1977) discussed the geochemical links between oil fields and ore deposits in sedimentary rocks with special reference to Alberta, and drew an analogy between the features of high salinity and high metal content of geothermal brines and the deeper, hotter, more saline formation waters from Alberta. A similarity was suggested between the leaching of hydrocarbons from shales to produce oil fields and the leaching of shales to produce enhanced contents of metals in formation waters, possibly resulting in ore deposits. This similarity is illustrated by the statistics presented above, in which data on Zn and Cl in formation waters (Hitchon et al., 1971), Zn in crude oils and Zn in shales are grouped according to the crude oil families distinguished by Deroo et al. (1977). In broad terms, the statistics may be summarized as follows:

	Group 1	Group 2	Group 3
Zn in shales	High	Intermediate	Low
Cl in formation waters	Low	Intermediate	High
Zn in formation waters	Low	Low	High
Zn in crude oils	Low	Intermediate	High
Hg in crude oils	Low	Low	High

It is tempting to speculate that the Zn in crude oils (and probably also Hg; see discussion in Hitchon and Filby, 1983, pp. 16-18) as well as Zn in formation waters, have originated from shales which yielded the crude oil hydrocarbons through the specific action of hot, chloride-rich formation waters, with the consequent depletion of those shales in Zn (and probably also Hg). The statistics on Cd in shales suggests little difference between the three groups, however.

A stepwise discriminant analysis of the shale composition data was carried out using logarithmic transforms where appropriate and the Wilk's lambda criterion for order of entry of the variables. Only Zn and Ca were significant discriminators, in order of their entry. Slightly more than 69% of the grouped samples were correctly classified. This result contrasts with that of Hitchon and Filby (1984) for grouped crude oils, where S, Co, Se, V and Br were the significant discriminators and 89.1% of the crude oils were correctly classified on the basis of their trace element content. The significance of these different results on shales and crude oils remains enigmatic.

Vanadium

General Statistics

V (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	7	46	87	86	127
Crude oils (n=20)	20	0.003	0.21	0.834	6.553
GROUP 2					
Shales (n=12)	12	55	75	116	421*
Crude oils (n=25)	23	0.068	20.88	28.1	138.8
GROUP 3					
Shales (n=7)	7	35	71	68	101
Crude oils (n=33)	32	0.014	1.0	6.28	52.67

*without this extreme value ($>3\sigma$ from the mean for all shales) the median, average and maximum values are 74, 88 and 165 ppm, respectively.

Geochemistry

The relation of V in Alberta shales and crude oils was discussed by Hitchon and Filby (1983, pp. 21-25), and will not be repeated here. Suffice to note there is some evidence to support the suggestion of a relation between the content of V in crude oils and the content of V in the source rocks.

Chromium

General Statistics

Cr (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	7	113	150	152	200
Crude oils (n=20)	7	0.00371	0.00780	0.00839	0.01551
Formation waters (n=15)	0	-	-	-	-
GROUP 2					
Shales (n=12)	12	116	160	162	228
Crude oils (n=25)	14	0.00466	0.245	0.0416	0.1058
Formation waters (n=25)	1	-	0.012	-	-
GROUP 3					
Shales (n=7)	7	44	101	114	221
Crude oils (n=33)	16	0.00363	0.0148	0.0326	0.2058
Formation waters (n=34)	3	0.016	0.016	0.022	0.034

Geochemistry

Little can be said about Cr in shales, crude oils and formation waters except that (1) there are no obvious trends among the groups, (2) Cr is very low in formation waters, (3) Cr is present in small amounts in just less than half the crude oils analysed, and (4) Cr occurs in fairly uniform amounts in most shales.

Manganese

General Statistics

Mn (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	7	74	221	284	740
Crude oils (n=20)	20	0.001	0.0506	0.0549	0.1192
Formation waters (n=15)	14	0.04	0.11	0.37	2.50
GROUP 2					
Shales (n=12)	12	104	241	310	921
Crude oils (n=25)	19	0.0017	0.0498	0.0471	0.07928
Formation waters (n=25)	22	0.09	0.33	0.53	3.18
GROUP 3					
Shales (n=7)	7	68	130	226	634
Crude oils (n=33)	31	0.01793	0.0492	0.0526	0.1766
Formation waters (n=34)	32	0.05	0.60	1.01	11.0

Geochemistry

Manganese was present in nearly all samples analysed. It formed a separate factor in the formation waters studied by Hitchon et al. (1971), and a separate factor in the crude oils studied by Hitchon et al. (1975). The above data on Mn in shales suggest fairly uniform contents in all shales without obvious differences among the three groups.

Iron, Cobalt and Nickel

General Statistics

Fe, Co, Ni (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	Fe 7	20100	36000	35400	45600
	Co 6	5	19	17	28
	Ni 7	66	170	147	200
Crude oils (n=20)	Fe 10	0.071	0.466	0.545	1.671
	Co 18	0.000261	0.00271	0.00803	0.02907
	Ni 15	0.022	0.520	0.939	4.03
Formation waters (n=15)	Fe 15	0.46	2.7	5.6	27.2
	Co 1	-	0.009	-	-
	Ni 2	0.047	0.057	0.057	0.066
GROUP 2					
Shales (n=12)	Fe 12	14000	32700	35200	81100*
	Co 11	2	12	17	42
	Ni 12	78	133	133	195
Crude oils (n=25)	Fe 12	0.286	0.587	0.94	2.19
	Co 25	0.000397	0.004484	0.0102	0.0622
	Ni 22	0.136	8.53	11.5	57.48
Formation waters (n=25)	Fe 25	0.05	0.94	6.6	54
	Co 3	0.005	0.008	0.014	0.029
	Ni 7	0.028	0.071	0.063	0.110
GROUP 3					
Shales (n=7)	Fe 7	2730	25200	26700	49000
	Co 6	2	16	22	48
	Ni 7	48	150	167	350**
Crude oils (n=33)	Fe 18	0.216	0.566	2.04	19.77
	Co 32	0.000516	0.00866	0.0227	0.2026
	Ni 24	0.085	3.51	7.96	70.1
Formation waters (n=34)	Fe 32	0.01	0.54	51	42
	Co 7	0.005	0.012	0.011	0.015
	Ni 5	0.026	0.042	0.038	0.046

* without this extreme value (>3σ from the mean for all shales) the median, average and maximum values are 32,000, 31,000 and 44,900 ppm, respectively.

** without this extreme value (>3σ from the mean for all shales) the median, average and maximum values are 140, 136 and 260 ppm, respectively.

Geochemistry

Iron, Co and Ni are present in nearly all shales, with Fe >> Ni > Co, with no significant differences between the groups except for slightly lower Fe in group 3 samples. Unlike the shales, the proportions in crude oils are Ni > Fe >> Co, with group 2 crude oils (which are heavy oils subjected to biodegradation and water washing) having enhanced contents of Ni. Although Fe is present in most formation waters, Co and Ni are seldom much above detection limits. Generally, there appears to be no relation among shales, crude oils and formation waters with respect to Fe, Co and Ni and the only differences among the groups related to lower Fe in group 3 shales and higher Ni in group 2 crude oils.

Copper and Silver

General Statistics

Cu, Ag (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	Cu 7	9	39	266	1600**
	Ag 3	1.2	1.3	16	44
Formation waters (n=15)	Cu 15	0.04	0.08	0.10	0.26
GROUP 2					
Shales (n=12)	Cu 12	21	31	34	70
	Ag 5	0.5	1.4	1.5	3.7
Formation waters (n=25)	Cu 25	0.05	0.11	0.14	0.44
GROUP 3					
Shales (n=7)	Cu 7	7	17	17	29
	Ag 5	0.5	2.4	4.8	16
Formation waters (n=34)	Cu 34	0.02	0.09	0.12	0.49

* without this extreme value (>3 σ from the mean for all shales) the median, average and maximum values are 35, 44 and 94, respectively.

Geochemistry

Copper is present in all shales and formation waters, and Ag in half the shales. Ignoring the extreme content of Cu (1600 ppm) in sample K-1, the general content of Cu decreases with depth from group 1 to group 3. In contrast, there is little difference in the distribution of Cu in formation waters among the groups. The Ag content of K-1 is 44 ppm and has biased the statistics for Ag in group 1. Generally, however, there appears to be little difference among the groups, bearing in mind Ag was below detection in half the shales.

Molybdenum

General Statistics

Mo (ppm or mg/l)	Number of samples reporting element	Minimum	Median	Average	Maximum
GROUP 1					
Shales (n=7)	7	7	21	21	32
GROUP 2					
Shales (n=12)	11	3	11	12	24
GROUP 3					
Shales (n=7)	6	10	16	21	54*

*without this extreme value ($>3\sigma$ from the mean for all shales) the median, average and maximum values are 12.5, 12.2 and 20 ppm, respectively.

Geochemistry

Molybdenum is found in nearly all shales. Even with the exception of sample K-10 (54 ppm Mo), there is no indication of significant differences among the groups.

Lead

General Statistics

Pb (ppm or mg/l)	Number of samples reporting element	% samples with Pb below detection	Minimum	Median	Average	Maximum
GROUP 1						
Shales (n=7)	7	0	5	10	17	55
GROUP 2						
Shales (n=12)	8	33	5	5	7	10
GROUP 3						
Shales (n=7)	0	100	-	-	-	-

Geochemistry

Lead presents possibly the clearest evidence of trace element differences between the shale groups, made more obvious in the above table by the addition of the column of percentage of samples with Pb below detection (~5 ppm). The most obvious reason for this difference is that Pb occurs dominantly as chloride complexes in saline formation waters and so can easily be mobilized from the shales by the deeper, more saline formation waters.

GEOCHEMISTRY OF KEROGEN

ELEMENTAL COMPOSITION

The raw elemental composition was adjusted for pyrite-S (% Fe x 1.1482) and ash, and normalized (Sum CHONS = 100). Orr (1986) showed that this method of adjusting for pyrite-S is in reasonable agreement with pyrite-S recovered by HNO₃ leaching.

When plotted (Figure 3B) on a van Krevelen diagram (atomic H/C against atomic O/C) the majority of samples are classed as Type III kerogen with three classed as Type II. Most fall in the zones of catagenesis and cracking (Figure 3A), i.e. the principal zone of oil formation and the zone of wet gas, respectively. Figure 3C shows the general environment of deposition of the shale from which the kerogen was extracted together with the estimated maximum temperature from Table 4. As expected, increased temperature results first in a rapid decrease in atomic O/C ratio (well seen in the non-marine Type III data), then a gradual decrease in the atomic H/C ratio for Type III kerogen or a rapid decrease in the atomic H/C ratio for Type II kerogen.

On a ternary diagram of the heteroatoms (NSO = 100 wt.%) most data plot in the O-rich portion of the diagram (Figure 4). According to the proposed criteria of Orr (1986), all the Alberta Basin kerogens except BH-431G (atomic S/C 0.0234) would be classed as low-S types (atomic S/C < 0.02). Maximum temperature data from Table 4 are also given in Figure 4, and there is a tendency for a relative decrease in O in kerogen with increasing temperature. The solid tie line and dashed tie line join up data from the Viking Formation and non-oilsand Mannville Group, respectively. These trends suggest a tendency for a loss of both O and S with increased temperature, and therefore a relative increase in N as a residual effect. Plots (not shown) of both atomic H/C vs atomic N/C and atomic H/C vs atomic S/C are relatively 'flat'.

ESR PROPERTIES

Three properties of the ESR signal were measured and are plotted against estimated maximum temperature in Figure 5A (broad band spins per gram), Figure 5B (g-value) and Figure 5C (broad band width). As expected, increased temperature results in increased spin concentrations, lower g-values, and wider lines. There seem to be distinct and separate trends for the Viking Formation and non-oilsand Mannville Group kerogens, with higher atomic H/C ratios (Figure 3B), higher relative amounts of O and lower relative amounts of S (Figure 4), and lower spin concentrations and g-values in the Viking Formation samples. The data are too few and the trends too tentative to do more than suggest the above relations.

¹³C NMR PROPERTIES

Figure 6 shows three typical ¹³C NMR spectra from kerogen samples analyzed in this study. The most useful parameter is the aliphatic-carbon/aromatic-carbon ratio, which

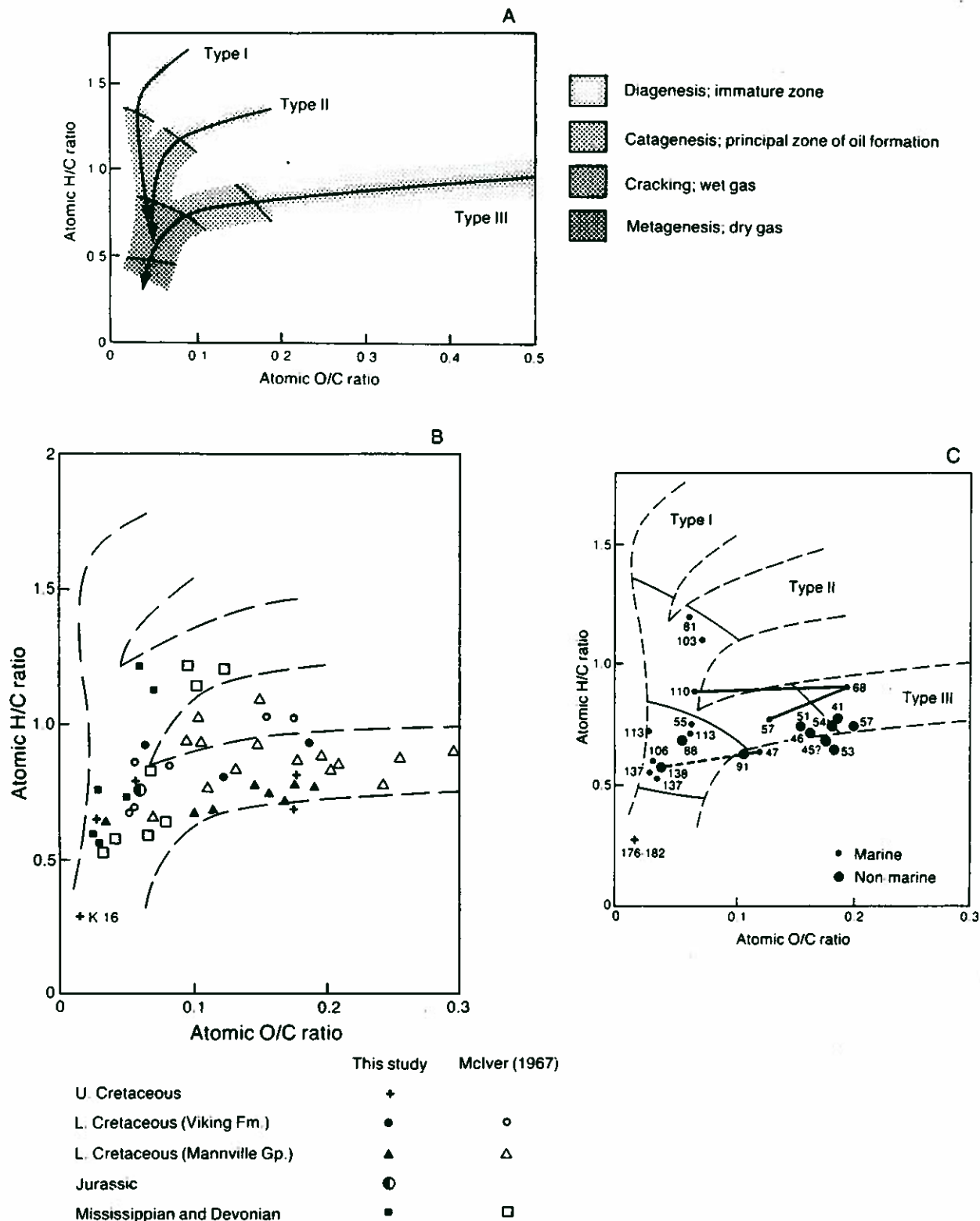


Figure 3. A. van Krevelan diagram (atomic H/C vs atomic O/C) showing maturation regions; B. van Krevelan diagram for kerogens from the Alberta Basin. The cross (+) is sample K-16 from the Middle Devonian Nahanni Formation of northeast British Columbia (4125 m, $R_o \sim 2.5$, estimated present reservoir temperature 180°C). C. van Krevelan diagram for kerogens from the Alberta Basin showing the general environment of deposition of the shales from which the kerogen was extracted, and the estimated maximum temperatures (°C). Solid tie line - Viking Formation; dashed tie line - non-oilsands Mannville Group.

Table 4. Estimated maximum burial depth and temperature.

Sample number	Present depth (m) [Appendix A]	Eroded thickness (m) [Hitchon, 1984 Fig. 23]	Paleogeothermal gradient (°C/km) [Hitchon, 1984 Fig. 24]	Maximum burial depth (km)	Maximum temperature (°C)
RCA 65-1	80	2050	25	2.1	53
RCA 67-1	140	1400	27	1.5	41
K-1	2145	2500	23	4.6	106
W-28	440	*2000	*23	2.4	55
K-2	620	1500	27	2.1	57
K-3	1040	1600	26	2.6	68
K-4	2190	2400	24	4.6	110
BH-431A	225	*1500	*27	1.7	46
BH-431G	425	*1500	*27	1.9	51
BH-427A	370	1450	26	1.8	47
BH-439A	440	*1600	*27	2.0	54
BH-433A	455	*1600	*27	2.1	57
BH-435F	300	?	?	-	*45
K-5	1485	2000	26	3.5	91
K-6	3375	2600	23	6.0	138
K-7	2535	2400	23	4.9	113
K-8	1980	*2100	*25	4.1	103
HE 32/35	3120	2600	24	5.7	137
HE 36	3120	2600	24	5.7	137
K-9	955	1500	26	2.5	65
K-10	1895	2050	25	3.9	98
K-11	1565	1450	27	3.0	81
K-12	2805	1700	25	4.5	113
K-13	1620	1750	26	3.4	88
K-15	2655	2000	25	4.7	118

* = estimated

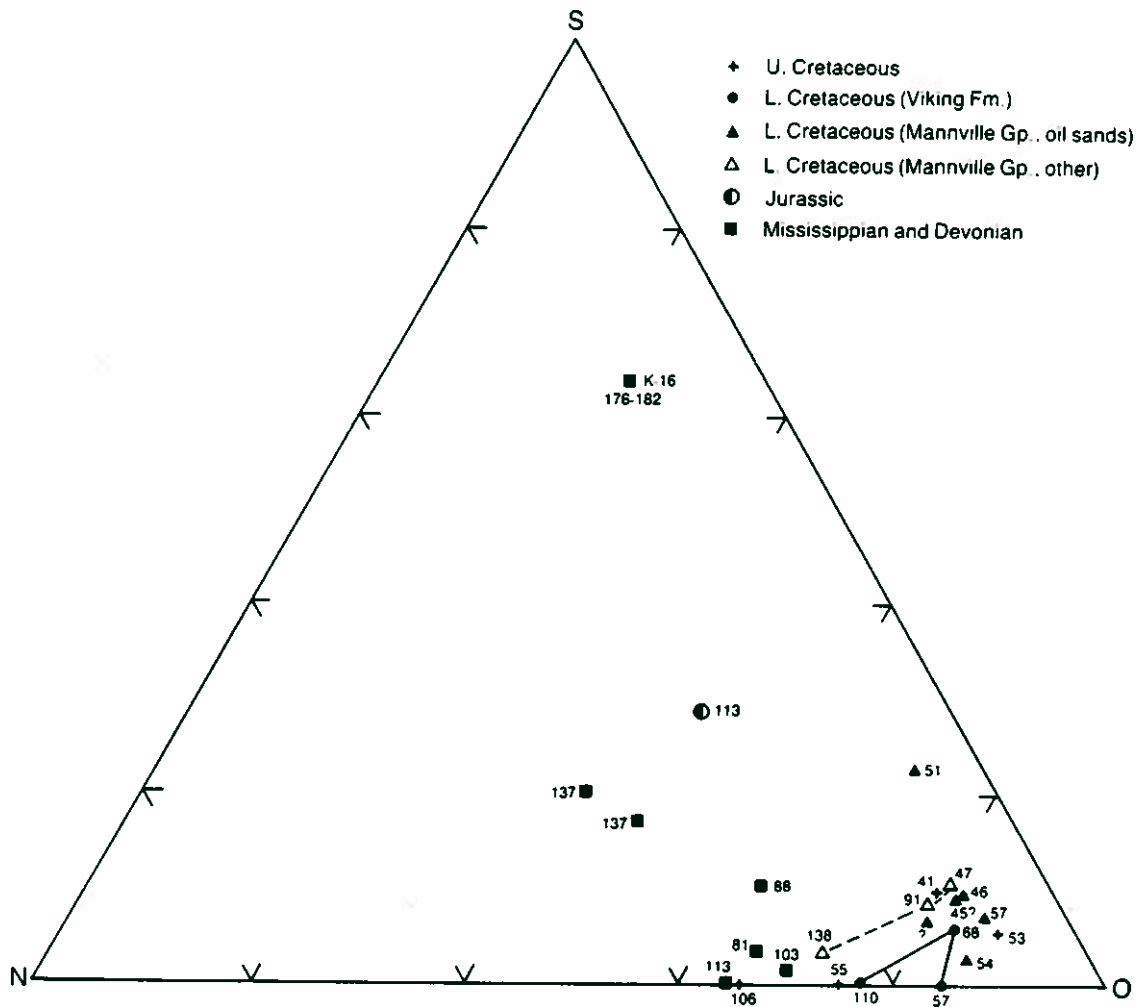


Figure 4. Ternary diagram of heteroatoms (NSO=100 wt.%) in kerogens from the Alberta Basin, showing stratigraphic unit and estimated maximum temperature (°C). For details of sample K-16 see caption to Figure 3. Solid tie line - Viking Formation; dashed tie line - non-oilsands Mannville Group.

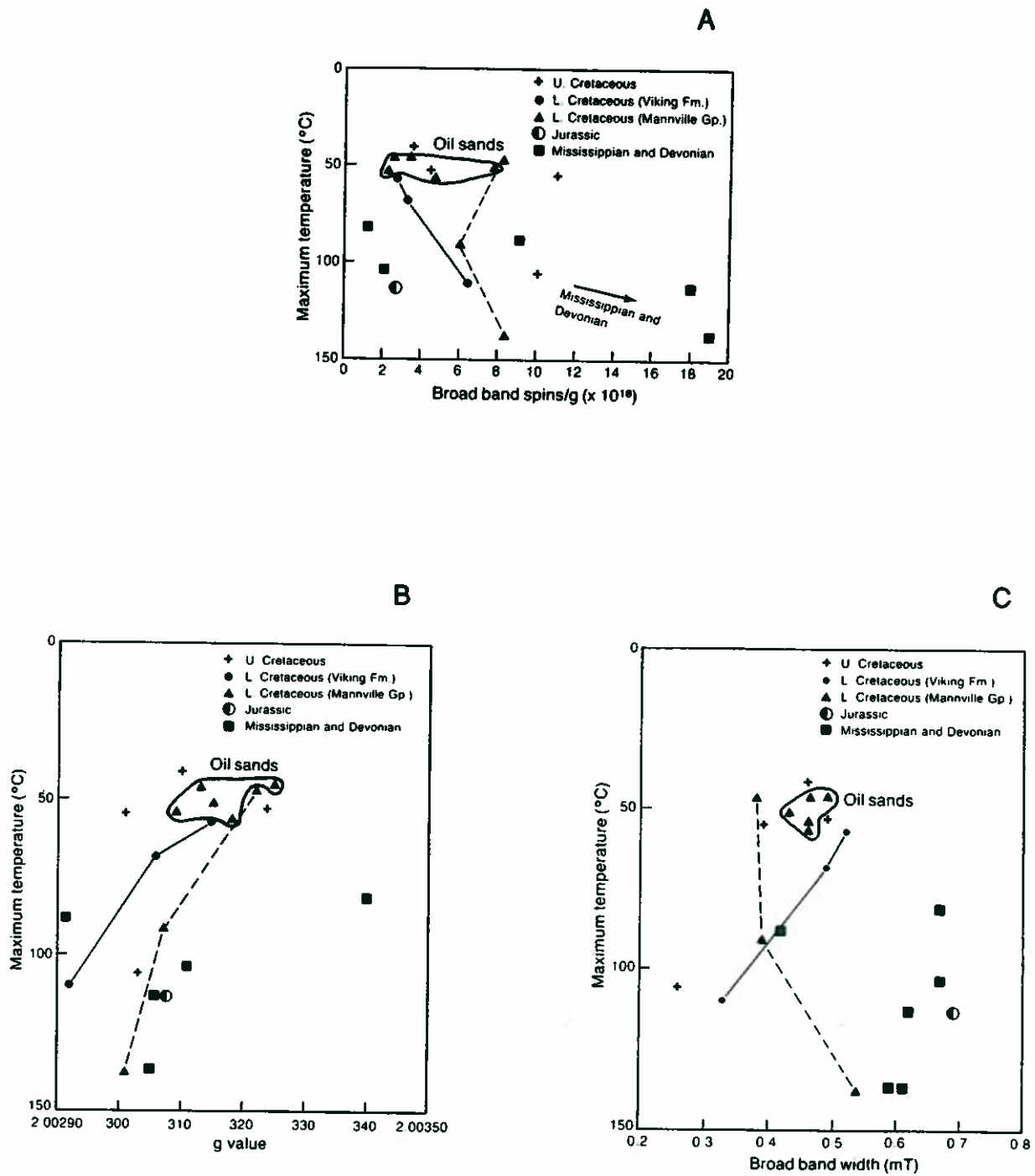


Figure 5. Relation of: A. ESR broad band spin concentration (spins/gx10¹⁸); B. ESR g-value; and C. ESR broad band width (mT) to estimated maximum temperature (°C) in kerogens from the Alberta Basin. Solid tie line - Viking Formation; dashed tie line - non-oilsands Mannville Group.

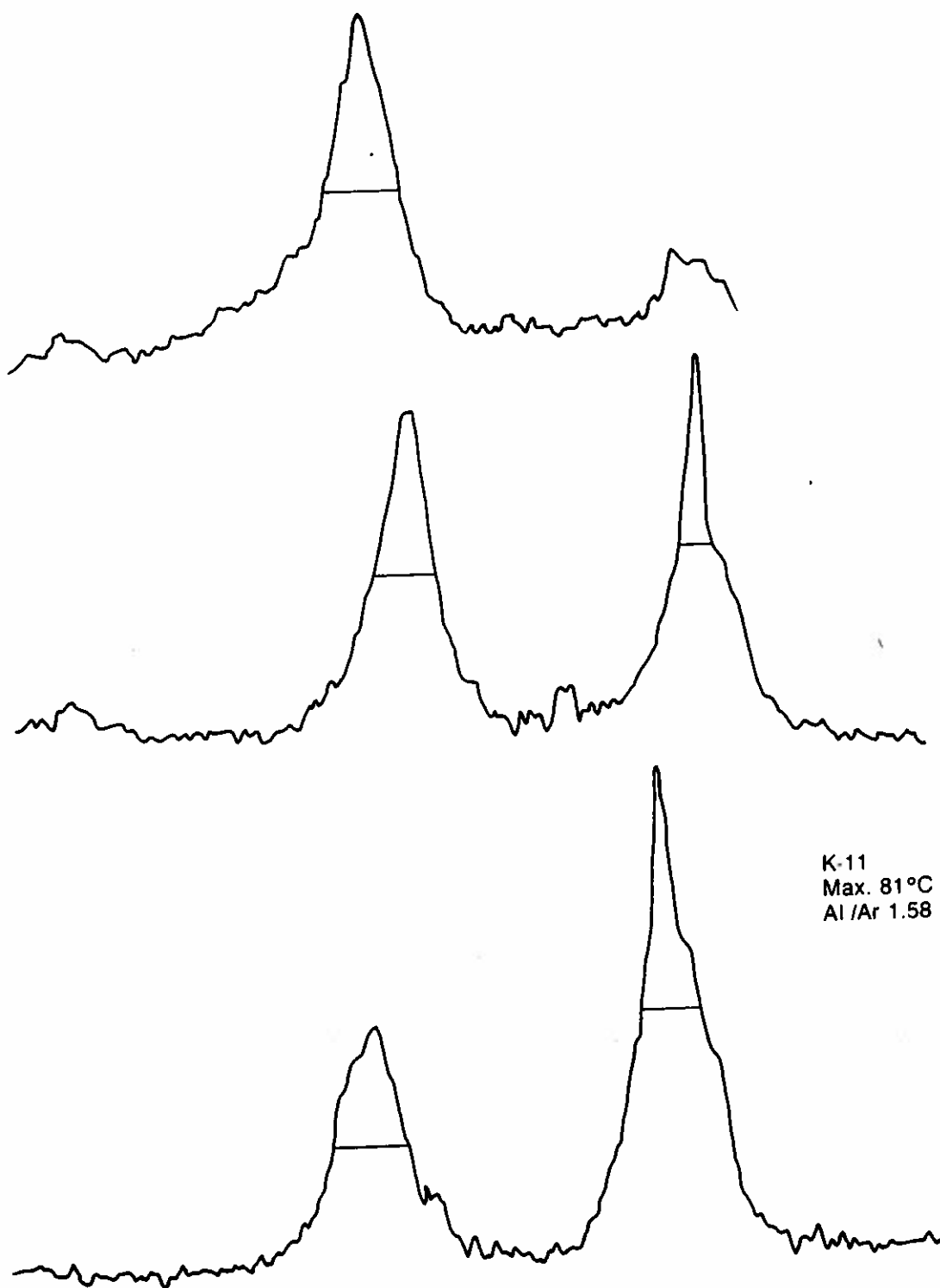


Figure 6. Typical ^{13}C NMR spectra from kerogen samples from the Alberta Basin.

reflects both the original chemical composition of the kerogen and a measure of the maturation to which it has been subjected. This ratio is reported in Table 5 for the samples studied. Figure 7 is a plot of the aliphatic/aromatic ratio against estimated maximum temperature. For the three samples from the Viking Formation increasing temperature results in generally decreased aliphatic/aromatic carbon ratio; this trend is not obvious for the other samples, and at any specific temperature there is a wide range of ratios.

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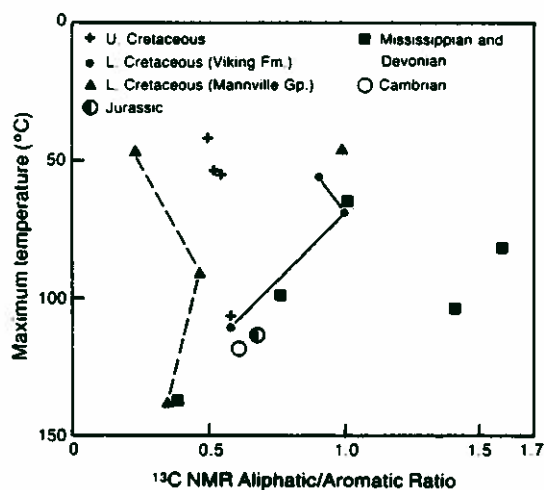


Figure 7. Relation of aliphatic-carbon/aromatic-carbon ratio and estimated maximum temperature ($^{\circ}\text{C}$) in kerogens from the Alberta Basin. Solid tie line - Viking Formation; dashed tie line - non-oilsands Mannville Group.

Table 5. ^{13}C NMR properties of kerogen extracted from Alberta Basin shales; for complete details of samples see Appendix A.

Sample number	^{13}C NMR properties	
	width (mT)	aliphatic/aromatic carbon ratio (corrected for spinning side bands)
RCA 65-1	0.49	0.52
RCA 67-1	0.46	0.50
K-1	0.26	0.58
W-28	0.39	0.54
K-2	0.52	0.92
K-3	0.49	1.00
K-4	0.33	0.58
BH-431A	0.49	-
BH-431G	0.43	-
BH-427A	0.38	0.23
BH-439A	0.46	-
BH-433A	0.46	-
BH-435F	0.46	0.99
K-5	0.39	0.47
K-6	0.54	0.35
K-7	0.69	0.67
RL 2/4	-	-
K-8	0.67	1.41
HE 32/35	0.61	0.38
HE 36	0.59	-
K-9	-	1.0
K-10	-	0.76
K-11	0.67	1.58
K-12	0.62	-
K-13	0.42	-
K-14	-	-
K-16	-	-
K-15	-	0.61

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APPENDIX A

Geochemistry of Alberta shales and associated kerogen

Data sheets

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 1

Sample number: RCA 65-1
 Stratigraphic unit: U. Cretaceous, Post-Colorado Supergroup, Edmonton Fm.
 Well name: RCA Corehole 65-1 (Wizard Lake)
 Location: 4-8-48-27-W4M Depth (m): 79.2-80.5
 Description: claystone, silty, grey, shaley partings
 Depositional environment: fresh to brackish water

MAJOR OXIDES (%)

SiO₂ 71
 TiO₂ 0.7
 Al₂O₃ 17
 Σ Fe as Fe₂O₃ 5.7
 MgO 2.0
 CaO 1.2
 Na₂O 0.7
 Σ 98.3

TRACE ELEMENTS (ppm)

Ag *
 Cd 14
 Co 26
 Cr 164
 Cu 70
 Mn 740
 Mo 21
 Ni 90
 Pb 10
 Sr 170
 V 87
 Zn 161

ORGANICS

Organic C (%) 1.116
 Extractable organics (ppm) 80.5
 R_s (average) 0.70

* = Below detection
 - = Not determined

ASSOCIATED KEROGEN

Normalized composition (Sum CHONS = 100)
 Adjusted for pyrite sulfur (%Fe x 1.1482)

C 75.30
 H 4.33
 O 17.77
 N 1.45
 S 1.15

Atomic H/C 0.685
 O/C 0.1771
 N/C 0.0164
 S/C 0.0057

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 4.5x10¹⁸
 g-value Narrow 2.00300
 Broad 2.00324
 width (mT) Narrow 0.13
 Broad 0.49

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -8.8
 Extractable organics -0.4
 Pyrite -

COMMENTS

For a description of the cored section see Snead (1969, pp. 74-80) and Carrigy (1971, pp. 97-100). Sample probably best described as a siltstone.

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 2

Sample number: RCA 67-1
 Stratigraphic unit: U.Cretaceous, Post-Colorado Supergroup, Bearpaw Fm.
 Well name: RCA Corehole No. 67-1 (Castor)
 Location: 13-34-37-13-W4M Depth (m) 137.8-141.1
 Description: medium to dark grey, bentonitic shale
 Depositional environment: marginal marine, quiet shallow water

MAJOR OXIDES (%)

SiO ₂	77
TiO ₂	0.6
Al ₂ O ₃	14
ΣFe as Fe ₂ O ₃	5.8
MgO	1.7
CaO	0.9
Na ₂ O	0.7
	Σ 100.7

TRACE ELEMENTS (ppm)

Ag	*
Cd	13
Co	26
Cr	149
Cu	39
Mn	301
Mo	32
Ni	120
Pb	10
Sr	170
V	98
Zn	154

ORGANICS

Organic C (%)	1.088
Extractable organics (ppm)	980
R _o (average)	0.68

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C	73.31
H	4.92
O	17.41
N	2.21
S	2.15

Atomic H/C	0.800
O/C	0.1783
N/C	0.0257
S/C	0.0110

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow	1.1x10 ¹⁶
Broad	3.6x10 ¹⁸
g-value Narrow	2.00280
Broad	2.00310
width (mT) Narrow	-
Broad	0.46

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen	-12.1
Extractable organics	-3.8
Pyrite	-7.9

COMMENTS

For a description of the well see Given and Wall (1971, p. 507; well log Fig. 2; microfaunal-microfloral associations Fig. 6).

Sample came from the middle of the Lower Shale Unit.

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 3

Sample number: K-1
 Stratigraphic unit: U.Cretaceous, U.Colorado Gp., Cardium Fm.
 Well name: Canadian Superior Los Nietos O'Chiese 9-11
 Location: 9-11-44-10-W5M Depth (m): 2137.6-2150.7
 Description: -
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 60
 TiO₂ 0.6
 Al₂O₃ 10
 ΣFe as Fe₂O₃ 4.3
 MgO 1.2
 CaO 0.4
 Na₂O 0.2
 Σ 76.7

TRACE ELEMENTS (ppm)

Ag 44
 Cd 13
 Co 5
 Cr 130
 Cu 1600
 Mn 164
 Mo 20
 Ni 180
 Pb 55
 Sr 64
 V 78
 Zn 943

ORGANICS

Organic C (%) 0.816
 Extractable organics (ppm) 1900
 R_o (average) 1.27

* = Below detection

- = Not determined

COMMENTS

Core 2, Box 4 of 10.

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 89.66
 H 4.75
 O 3.69
 N 1.90
 S 0.00

Atomic H/C 0.631
 O/C 0.0309
 N/C 0.0181
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 1.0x10¹⁹
 g-value Narrow 2.00268
 Broad 2.00303
 width (mT) Narrow -
 Broad 0.26

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -5.1
 Pyrite -

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 4

Sample number: W-28
 Stratigraphic unit: U.Cretaceous, U.Colorado Gp., Kaskapau Fm.
 Doe Creek Ss.
 Well name: Pacific Inland PCoupeS 9-5DC-78-12
 Location: 9-5-78-12-W6M Depth (m): 440.4-443.5
 Description:
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 60
 TiO₂ 0.9
 Al₂O₃ 18
 ΣFe as Fe₂O₃ 5.1
 MgO 1.5
 CaO 0.4
 Na₂O 0.4
 Σ 86.3

TRACE ELEMENTS (ppm)

Ag 1.2
 Cd 11
 Co 11
 Cr 200
 Cu 94
 Mn 192
 Mo 7
 Ni 66
 Pb 15
 Sr 113
 V 127
 Zn 206

ORGANICS

Organic C (%) 1.400

Extractable

organics (ppm) 2780

R_o (average) -

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS=100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 85.46
 H 5.52
 O 6.79
 N 2.23
 S 0.00

Atomic H/C 0.770

O/C 0.0596

N/C 0.0223

S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 1.5x10¹⁷

Broad 1.1x10¹⁹

g-value Narrow 2.00279

Broad 2.00301

width (mT) Narrow -

Broad 0.39

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen +19.7

Extractable organics +16.6

Pyrite +29.0

COMMENTS

δ¹⁸O (‰ SMOW) = +18.5 on carbonate cement from adjacent sandstone (Hitchon and Friedman, 1969, p. 1344, sample No. 28).

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 5

Sample number: K-2
 Stratigraphic unit: L.Cretaceous, L.Colorado Gp., Viking Fm.
 Well name: Imperial Pinedale No. 1
 Location: 7-28-54-16-W4M Depth (m): 602.0-604.7
 633.4-635.5
 Description: medium grey shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 68
 TiO₂ 0.7
 Al₂O₃ 17
 Σ Fe as Fe₂O₃ 6.5
 MgO 2.0
 CaO 0.4
 Na₂O 0.5
 Σ 95.1

TRACE ELEMENTS (ppm)

Ag *
 Cd 24
 Co 5
 Cr 150
 Cu 23
 Mn 221
 Mo 26
 Ni 200
 Pb 15
 Sr 180
 V 66
 Zn 145

ORGANICS

Organic C (%) 1.176
 Extractable organics (ppm) 1030
 R_o (average) 0.79

* = Below detection
 - = Not determined

COMMENTS

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 79.29
 H 5.38
 O 13.03
 N 2.30
 S 0.00

Atomic H/C 0.808
 O/C 0.1234
 N/C 0.0247
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 2.8x10¹⁸
 g-value Narrow 2.00289
 Broad 2.00315
 width (mT) Narrow -
 Broad 0.52

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -11.1
 Extractable organics -4.8
 Pyrite -14.8

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 6

Sample number: K-3
 Stratigraphic unit: L.Cretaceous, L.Colorado Gp., Viking Fm.
 Well name: Imp Home Duhamel 4-8-46-21
 Location: 4-8-46-21-W4M Depth (m): 1038.5-1040.0
 Description: medium grey shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO ₂	71
TiO ₂	0.8
Al ₂ O ₃	15
ΣFe as Fe ₂ O ₃	5.1
MgO	1.6
CaO	0.3
Na ₂ O	0.6
	Σ 94.4

TRACE ELEMENTS (ppm)

Ag	*
Cd	26
Co	28
Cr	160
Cu	30
Mn	297
Mo	28
Ni	200
Pb	10
Sr	183
V	102
Zn	180

ORGANICS

Organic C (%)	1.460
Extractable organics (ppm)	815
R _o (average)	0.70

* = Below detection
 - = Not determined

COMMENTS

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C	72.58
H	5.71
O	18.10
N	2.34
S	1.27

Atomic H/C	0.937
O/C	0.1872
N/C	0.0275
S/C	0.0066

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow	-
Broad	3.3x10 ¹⁸
g-value Narrow	2.00277
Broad	2.00306
width (mT) Narrow	-
Broad	0.49

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen	-7.2
Extractable organics	-1.6
Pyrite	+2.3

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 7

Sample number: K-4
 Stratigraphic unit: L.Cretaceous, L.Colorado Gp., Viking Fm.
 Well name: Oilwell Operators et al. Alhambra 16-11
 Location: 16-11-38-5-W5M Depth (m): 2188.5-2190.0
 Description: medium grey shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 56
 TiO₂ 0.5
 Al₂O₃ 9
 ΣFe as Fe₂O₃ 2.9
 MgO 1.2
 CaO 0.5
 Na₂O 0.1
 Σ 70.2

TRACE ELEMENTS (ppm)

Ag 1.3
 Cd 6.4
 Co *
 Cr 113
 Cu 9
 Mn 74
 Mo 10
 Ni 170
 Pb 5
 Sr 62
 V 46
 Zn 99

ORGANICS

Organic C (%) 1.092
 Extractable organics (ppm) 2090
 R_o (average) 0.88

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 84.33
 H 6.52
 O 7.10
 N 2.05
 S 0.00

Atomic H/C 0.921
 O/C 0.0632
 N/C 0.0207
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 6.4x10¹⁸
 g-value Narrow 2.00287
 Broad 2.00292
 width (mT) Narrow -
 Broad 0.33

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen +6.1
 Extractable organics +12.1
 Pyrite +2.8

COMMENTS

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 8

Sample number: BH-431A
 Stratigraphic unit: L.Cretaceous, Grand Rapids Fm.
 Well name: BA Wabasca 10-25-81-22
 Location: 10-25-81-22-W4M Depth (m): 222.5-226.8
 Description: medium to dark grey, slightly silty shale
 Depositional environment: non-marine

MAJOR OXIDES (%)

SiO ₂	71
TiO ₂	0.8
Al ₂ O ₃	18
ΣFe as Fe ₂ O ₃	5.4
MgO	2.2
CaO	0.3
Na ₂ O	0.6
	Σ 98.3

TRACE ELEMENTS (ppm)

Ag	*
Cd	14
Co	2
Cr	140
Cu	21
Mn	297
Mo	7
Ni	101
Pb	10
Sr	207
V	59
Zn	150

ORGANICS

Organic C (%)	0.900
Extractable organics (ppm)	555
R _o (average)	-

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C	75.53
H	4.75
O	15.85
N	2.59
S	1.28

Atomic H/C	0.749
O/C	0.1575
N/C	0.0292
S/C	0.0063

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow	-
Broad	2.6x10 ¹⁸
g-value Narrow	-
Broad	2.00313
width (mT) Narrow	-
Broad	0.49

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen	-16.5
Extractable organics	-
Pyrite	-28.2

COMMENTS

Wabasca (Grand Rapids A) oil sand deposit; composite of 13 samples over interval 222.5-226.8 m.

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 9

Sample number: BH-431G
 Stratigraphic unit: L.Cretaceous, Clearwater Fm., Wabiskaw Mbr.
 Well name: BA Wabasca 10-25-81-22
 Location: 10-25-81-22-W4M Depth (m): 425.5-427.9
 Description: carbonaceous shale above coal
 Depositional environment: non-marine

MAJOR OXIDES (%)

SiO₂ 45
 TiO₂ 0.6
 Al₂O₃ 15
 ΣFe as Fe₂O₃ 4.2
 MgO 0.9
 CaO 0.6
 Na₂O 0.1
 Σ 66.4

TRACE ELEMENTS (ppm)

Ag *
 Cd 10
 Co 8
 Cr 158
 Cu 29
 Mn 231
 Mo 6
 Ni 78
 Pb *
 Sr 95
 V 59
 Zn 127

ORGANICS

Organic C (%) 2.020
 Extractable organics (ppm) 2070
 R_o (average) 0.67

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 74.67
 H 4.85
 O 14.58
 N 1.24
 S 4.66

Atomic H/C

0.774

O/C

0.1466

N/C

0.0142

S/C

0.0234

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 7.8x10¹⁶
 Broad 7.9x10¹⁸
 g-value Narrow 2.00295
 Broad 2.00315
 width (mT) Narrow -
 Broad 0.43

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen +18.5
 Extractable organics +24.1
 Pyrite +21.7

COMMENTS

Wabasca oil sand deposit; composite of 10 samples over sampled interval.

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 10

Sample number: BH-427A
 Stratigraphic unit: L.Cretaceous, Clearwater Fm.
 Well name: Union Red Earth 10-14-88-9
 Location: 10-14-88-9-W5M Depth (m): 365.2-379.5
 Description: medium grey shale with pyrite nodules
 Depositional environment: marine

MAJOR OXIDES (%)

SiO ₂	49
TiO ₂	0.6
Al ₂ O ₃	13
ΣFe as Fe ₂ O ₃	11.6
MgO	4.7
CaO	4.4
Na ₂ O	0.1
	Σ 83.4

TRACE ELEMENTS (ppm)

Ag	0.5
Cd	22
Co	11
Cr	228
Cu	40
Mn	921
Mo	21
Ni	159
Pb	*
Sr	333
V	145
Zn	261

ORGANICS

Organic C (%)	0.844
Extractable organics (ppm)	865
R _o (average)	-

* = Below detection

- = Not determined

COMMENTS

Loon River oil sand deposit.

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C	79.83
H	4.59
O	12.48
N	1.54
S	1.56

Atomic H/C	0.685
O/C	0.1173
N/C	0.0165
S/C	0.0073

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow	-
Broad	8.2x10 ¹⁸
g-value Narrow	2.00284
Broad	2.00322
width (mT) Narrow	-
Broad	0.38

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen	-
Extractable organics	-
Pyrite	-

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 11

Sample number: BH-439A
 Stratigraphic unit: L. Cretaceous, U. Grand Rapids Fm.
 Well name: Pan Am A1 Michel Lake 10-25-58-5
 Location: 10-25-58-5-W4M Depth (m): 441.4-443.2
 Description: light to medium gray, fissile to blocky shale
 Depositional environment: non-marine

MAJOR OXIDES (%)

SiO₂ 62
 TiO₂ 0.8
 Al₂O₃ 19
 ΣFe as Fe₂O₃ 4.6
 MgO 2.1
 CaO 0.5
 Na₂O 0.4
 Σ 89.4

TRACE ELEMENTS (ppm)

Ag 1.4
 Cd 13
 Co 11
 Cr 217
 Cu 32
 Mn 423
 Mo 7
 Ni 113
 Pb 10
 Sr 121
 V 63
 Zn 109

ORGANICS

Organic C (%) 0.432
 Extractable organics (ppm) 895
 R_o (average) -

* = Below detection

- = Not determined

COMMENTS

Cold Lake oil sand deposit.

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 74.58
 H 4.88
 O 17.62
 N 2.37
 S 0.55

Atomic H/C 0.780
 O/C 0.1773
 N/C 0.0271
 S/C 0.0028

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 2.3x10¹⁸
 g-value Narrow -
 Broad 2.00309
 width (mT) Narrow -
 Broad 0.46

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -
 Pyrite -

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 12

Sample number: BH-433A
 Stratigraphic unit: L.Cretaceous, Mannville Gp.
 Well name: Imp 73-5 Leming OV 13-33-64-3
 Location: 13-33-64-3-W4M Depth (m): 454.5-458.3
 Description: dark grey, slightly silty shale
 Depositional environment: non-marine

MAJOR OXIDES (%)

SiO₂ 45
 TiO₂ 0.6
 Al₂O₃ 13
 ΣFe as Fe₂O₃ 6.4
 MgO 1.7
 CaO 0.4
 Na₂O 0.7
 Σ 67.8

TRACE ELEMENTS (ppm)

Ag *
 Cd 13
 Co 12
 Cr 172
 Cu 32
 Mn 250
 Mo 11
 Ni 78
 Pb *
 Sr 202
 V 59
 Zn 109

ORGANICS

Organic C (%) 3.924
 Extractable organics (ppm) 9550
 R_o (average) 0.61

* = Below detection
 - = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 73.41
 H 4.76
 O 18.64
 N 1.74
 S 1.45

Atomic H/C 0.773
 O/C 0.1906
 N/C 0.0202
 S/C 0.0074

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 2.6x10¹⁶
 Broad 4.7x10¹⁸
 g-value Narrow 2.00285
 Broad 2.00318
 width (mT) Narrow -
 Broad 0.46

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -8.7
 Extractable organics +3.6
 Pyrite -16.0

COMMENTS

Cold Lake oil sand deposit (Lower Grand Rapids Fm.).

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 13

Sample number: BH 435-F
 Stratigraphic unit: L. Cretaceous, McMurray Fm.
 Well name: Shell Eils OV 6-25-95-16
 Location: 6-25-95-16-W4M Depth (m): 301.1-301.4
 Description: dark grey fissile shale
 Depositional environment: freshwater deltaic

MAJOR OXIDES (%)

SiO₂ 64
 TiO₂ 0.7
 Al₂O₃ 22
 ΣFe as Fe₂O₃ 3.4
 MgO 1.0
 CaO 0.2
 Na₂O 0.3
 Σ 91.6

TRACE ELEMENTS (ppm)

Ag *
 Cd 10
 Co 11
 Cr 161
 Cu 32
 Mn 104
 Mo 3
 Ni 95
 Pb 5
 Sr 113
 V 76
 Zn 99

ORGANICS

Organic C (%) 4.912
 Extractable organics (ppm) 3810
 R_o (average) -

* = Below detection

- = Not determined

COMMENTS

Athabasca oil sand deposit

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 74.82
 H 4.46
 O 17.01
 N 1.79
 S 1.92

Atomic H/C 0.710
 O/C 0.1707
 N/C 0.0204
 S/C 0.0096

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 4.0x10¹⁸
 g-value Narrow 2.00288
 Broad 2.00325
 width (mT) Narrow -
 Broad 0.46

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics +20.7
 Pyrite +23.1

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 14

Sample number: K-5
 Stratigraphic unit: L.Cretaceous, U.Mannville Gp.
 Well name: Anglo Canadian Wabamun No. 1
 Location: 5-10-51-4-W5M Depth (m): 1481.6-1484.7
 Description: -
 Depositional environment: fluvial-lagoonal (Luscar facies; see Mellon (1967))

MAJOR OXIDES (%)

SiO₂ 58
 TiO₂ 0.8
 Al₂O₃ 14
 ΣFe as Fe₂O₃ 4.3
 MgO 2.0
 CaO 0.5
 Na₂O 0.6
 Σ 80.2

TRACE ELEMENTS (ppm)

Ag *
 Cd 16
 Co 14
 Cr 140
 Cu 70
 Mn 620
 Mo 20
 Ni 180
 Pb 5
 Sr 120
 V 74
 Zn 166

ORGANICS

Organic C (%) 1.656
 Extractable organics (ppm) 3520
 R_o (average) 0.50

* = Below detection
 - = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 81.49
 H 4.59
 O 11.10
 N 1.68
 S 1.14

Atomic H/C 0.671
 O/C 0.1022
 N/C 0.0176
 S/C 0.0052

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 6.0x10¹⁸
 g-value Narrow 2.00284
 Broad 2.00307
 width (mT) Narrow -
 Broad 0.39

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics +2.9
 Pyrite -

COMMENTS

For a description of the lithology, fossil content and facies of this well see Mellon (1967, Figs. 11 and 13).

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 15

Sample number: K-6
 Stratigraphic unit: L.Cretaceous, L.Blairmore Gp.
 Well name: Triad BA Stolberg 6-10A
 Location: 6-10-42-15-W5M
 Description: -
 Depositional environment: fluvialite (Mountain Park facies); see Mellon (1967)
 Depth (m): 3374.4-3375.1

MAJOR OXIDES (%)

SiO₂ 64
 TiO₂ 0.5
 Al₂O₃ 11
 ΣFe as Fe₂O₃ 4.8
 MgO 0.8
 CaO 0.9
 Na₂O 0.1
 Σ 82.1

TRACE ELEMENTS (ppm)

Ag *
 Cd 14
 Co 42
 Cr 120
 Cu 29
 Mn 121
 Mo *
 Ni 150
 Pb 5
 Sr 111
 V 93
 Zn 124

ORGANICS

Organic C (%) 2.068
 Extractable organics (ppm) 2020
 R_o (average) 0.47

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 89.56
 H 4.74
 O 4.10
 N 1.40
 S 0.20

Atomic H/C 0.631
 O/C 0.0344
 N/C 0.0133
 S/C 0.0008

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 3.0x10¹⁶
 Broad 8.4x10¹⁸
 g-value Narrow 2.00272
 Broad 2.00301
 width (mT) Narrow 0.11
 Broad 0.54

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen +9.5
 Extractable organics +6.6
 Pyrite +9.4

COMMENTS

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 16

Sample number: K-7
 Stratigraphic unit: L. Jurassic, Fernie Gp., Poker Chip Shale
 Well name: Union Condor 10-32-39-6
 Location: 10-32-39-6-W5M Depth (m): 2535.0-2539.9
 Description: medium grey, silty shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 64
 TiO₂ 0.8
 Al₂O₃ 18
 ΣFe as Fe₂O₃ 4.8
 MgO 3.1
 CaO 2.8
 Na₂O 0.0
 Σ 93.5

TRACE ELEMENTS (ppm)

Ag 0.5
 Cd 13
 Co 42
 Cr 165
 Cu 29
 Mn 408
 Mo 18
 Ni 130
 Pb 5
 Sr 198
 V 55
 Zn 65

ORGANICS

Organic C (%) 0.680
 Extractable organics (ppm) 1650
 R_o (average) -

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 81.28
 H 5.23
 O 6.45
 N 3.22
 S 3.82

Atomic H/C

0.767
 O/C 0.0596
 N/C 0.0338
 S/C 0.0176

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 1.0x10¹⁷
 Broad 2.7x10¹⁸
 g-value Narrow 2.00277
 Broad 2.00307
 width (mT) Narrow 0.03
 Broad 0.69

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -
 Pyrite -

COMMENTS

For details of the core from this well see Deere and Bayliss (1969)

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 17

Sample number: RL 2/4
 Stratigraphic unit: Mississippian, Banff Fm.
 Well name: Imperial Rainbow Lake 16-18-107-6
 Location: 16-18-107-6-W6M Depth (m): 542.7-546.9
 Description: medium dark grey shale (alternating with light grey limestone with scattered brachiopods)
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 81(?)
 TiO₂ 1.2
 Al₂O₃ 21
 ΣFe as Fe₂O₃ 5.0
 MgO 2.6
 CaO 2.2
 Na₂O 0.4
 Σ 113.4?

TRACE ELEMENTS (ppm)

Ag 1.4
 Cd 15
 Co 17
 Cr 200
 Cu 40
 Mn 110
 Mo 7
 Ni 136
 Pb *
 Sr 224
 V 121
 Zn 120

ORGANICS

Organic C (%) 0.604
 Extractable organics (ppm) 1220
 R_s (average) -

* = Below detection
 - = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 79.24
 H 5.23
 O 13.69
 N 1.84
 S 0.00

Atomic H/C 0.786
 O/C 0.1297
 N/C 0.0198
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 7.7x10¹⁸
 g-value Narrow -
 Broad 2.00294
 width (mT) Narrow -
 Broad 0.48

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -13.0
 Extractable organics -
 Pyrite -13.7

COMMENTS

Sum of CHONS of kerogen analysis very low (35.35%) and data should not be used in kerogen studies

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 18

Sample number: K-8
 Stratigraphic unit: Mississippian, Banff Fm.
 Well name: Shell BA Whitelaw No. 1
 Location: 2-14-82-2-W6M Depth (m): 1964.7-1971.4
 1986.1-1990.0
 Description: medium grey slightly calcareous shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 51
 TiO₂ 0.4
 Al₂O₃ 10
 ΣFe as Fe₂O₃ 3.9
 MgO 1.9
 CaO 2.3
 Na₂O 0.0
 Σ 69.5

TRACE ELEMENTS (ppm)

Ag *
 Cd 12
 Co 19
 Cr 116
 Cu 26
 Mn 120
 Mo 24
 Ni 150
 Pb 10
 Sr 46
 V 165
 Zn 156

ORGANICS

Organic C (%) 2.744
 Extractable organics (ppm) 4140
 R_o (average) -

* = Below detection
 - = Not determined

COMMENTS

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 81.39
 H 7.68
 O 7.58
 N 3.14
 S 0.21

Atomic H/C 1.124
 O/C 0.0699
 N/C 0.0329
 S/C 0.0010

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 2.0x10¹⁶
 Broad 2.0x10¹⁸
 g-value Narrow 2.00283
 Broad 2.00311
 width (mT) Narrow 0.10
 Broad 0.67

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -15.2
 Extractable organics -5.8
 Pyrite -16.6

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 19

Sample number: HE 32/35
 Stratigraphic unit: Mississippian, Exshaw Fm.
 Well name: Home Oil et al. C and E Elkton 7-3
 Location: 7-3-31-4-W5M Depth (m): 3118.4-3120.3
 Description: very dark grey to black shale, with (?) conodonts
 Depositional environment: marine (euxinic)

MAJOR OXIDES (%)

SiO₂ 47
 TiO₂ 0.3
 Al₂O₃ 8
 ΣFe as Fe₂O₃ 2.0
 MgO 2.2
 CaO >9.2
 Na₂O 0.0
 Σ >68.7

TRACE ELEMENTS (ppm)

Ag 3.7
 Cd 10
 Co *
 Cr 126
 Cu 29
 Mn 115
 Mo 12
 Ni 195
 Pb *
 Sr 352
 V 421
 Zn 155

ORGANICS

Organic C (%) 2.748
 Extractable organics (ppm) 3380
 R_o (average) 0.66

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 88.42
 H 4.39
 O 2.98
 N 2.75
 S 1.46

Atomic H/C 0.592
 O/C 0.0253
 N/C 0.0265
 S/C 0.0062

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow 1.1x10¹⁶
 Broad 1.9x10¹⁹
 g-value Narrow 2.00265
 Broad 2.00305
 width (mT) Narrow 0.098
 Broad 0.61

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen +10.3
 Extractable organics +1.7
 Pyrite +6.7

COMMENTS

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 20

Sample number: HE 36
 Stratigraphic unit: U.Devonian, Wabamun Gp.
 Well name: Home Oil et al. C and E Elkton 7-3
 Location: 7-3-31-4-W5M Depth (m): 3120.5-3123.0
 Description: dark grey shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 56
 TiO₂ 0.3
 Al₂O₃ 11
 ΣFe as Fe₂O₃ 4.4
 MgO 2.5
 CaO 9.1
 Na₂O 0.1
 Σ 83.4

TRACE ELEMENTS (ppm)

Ag *
 Cd 14
 Co 2
 Cr 93
 Cu 29
 Mn 130
 Mo 20
 Ni 159
 Pb *
 Sr 162
 V 71
 Zn 100

ORGANICS

Organic C (%) 2.792
 Extractable organics (ppm) 1540
 R_o (average) 0.67

* = Below detection

- = Not determined

COMMENTS

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 87.98
 H 4.16
 O 3.77
 N 2.73
 S 1.36

Atomic H/C 0.563
 O/C 0.0322
 N/C 0.0265
 S/C 0.0058

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 1.9x10¹⁹
 g-value Narrow 2.00262
 Broad 2.00305
 width (mT) Narrow 0.05
 Broad 0.59

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -10.7
 Extractable organics -5.6
 Pyrite -6.0

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 21

Sample number: K-9
 Stratigraphic unit: U.Devonian, Woodbend Gp., Ireton Fm. (middle unit)
 Well name: Socony Vegreville No. 1
 Location: 14-20-51-15-W4M Depth (m): 943.7-963.2
 Description: green-grey, calcareous shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 39
 TiO₂ 0.3
 Al₂O₃ 9
 ΣFe as Fe₂O₃ 3.3
 MgO 2.6
 CaO 3.2
 Na₂O 0.5
 Σ 57.9

TRACE ELEMENTS (ppm)

Ag 2.4
 Cd 14
 Co 16
 Cr 104
 Cu 23
 Mn 394
 Mo *
 Ni 130
 Pb *
 Sr 279
 V 38
 Zn 60

ORGANICS

Organic C (%) 0.180
 Extractable organics (ppm) 275
 R_o (average) -

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C -
 H -
 O -
 N -
 S -

Atomic H/C -
 O/C -
 N/C -
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad -
 g-value Narrow -
 Broad -
 width (mT) Narrow -
 Broad -

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -
 Pyrite -

COMMENTS

For the composition and mineralogy of the core from this well see Campbell and Oliver (1968).

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 22

Sample number: K-10
 Stratigraphic unit: U.Devonian, Woodbend Gp., Ireton Fm. (upper unit)
 Well name: Texaco Wizard Lake A-1
 Location: 14-14-48-27-W4M Depth (m): 1889.8-1899.2
 Description: green-grey, calcareous shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 60
 TiO₂ 0.6
 Al₂O₃ 16
 ΣFe as Fe₂O₃ 5.0
 MgO 3.3
 CaO 3.2
 Na₂O 0.1
 Σ 88.2

TRACE ELEMENTS (ppm)

Ag 16
 Cd 16
 Co 48
 Cr 149
 Cu 23
 Mn 634
 Mo 54
 Ni 150
 Pb *
 Sr 658
 V 101
 Zn 77

ORGANICS

Organic C (%) 0.204
 Extractable organics (ppm) 280
 R_o (average) -

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C -
 H -
 O -
 N -
 S -

Atomic H/C -
 O/C -
 N/C -
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad -
 g-value Narrow -
 Broad -
 width (mT) Narrow -
 Broad -

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -
 Pyrite -

COMMENTS

For the composition and mineralogy of the core from this well see Campbell and Oliver (1968).

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 23

Sample number: K-11
 Stratigraphic unit: U.Devonian, Woodbend Gp., Majeau Lake Fm.
 Well name: Imp Westlock 14-24-59-26
 Location: 14-24-59-26-W4M Depth(m) 1562.4-1567.9
 Description: black, bituminous, slightly calcareous shale
 Depositional environment: marine, close to carbonate reef complex

MAJOR OXIDES (%)

SiO ₂	56
TiO ₂	0.4
Al ₂ O ₃	12
ΣFe as Fe ₂ O ₃	3.6
MgO	1.3
CaO	3.4
Na ₂ O	0.0
	Σ76.7

TRACE ELEMENTS (ppm)

Ag	2.8
Cd	2.1
Co	39
Cr	101
Cu	7
Mn	204
Mo	18
Ni	70
Pb	*
Sr	182
V	84
Zn	46

ORGANICS

Organic C (%)	5.764
Extractable	
organics (ppm)	36,600
R _o (average)	0.33

* = Below detection
 - = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C	81.92
H	8.43
O	6.36
N	2.94
S	0.35

Atomic H/C	1.226
O/C	0.0583
N/C	0.0306
S/C	0.0016

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow	
Broad	1.2x10 ¹⁶
g-value Narrow	2.00295
Broad	2.00340
width (mT) Narrow	-
Broad	0.67

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen	+7.4
Extractable organics	+13.9
Pyrite	+11.8

COMMENTS

For a description of this type section see Pollock (1967)

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 24

Sample number: K-12
 Stratigraphic unit: U.Devonian, Beaverhill Lake Gp.
 Well name: Home Regent "B" Swan Hills 4-4-67-11
 Location: 4-4-67-11-W5M Depth (m): 2805.4-2809.2
 Description: medium grey calcareous shale
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 66
 TiO₂ 0.1
 Al₂O₃ 3
 ΣFe as Fe₂O₃ 0.4
 MgO 0.7
 CaO >9.2
 Na₂O 0.1
 Σ >79.5

TRACE ELEMENTS (ppm)

Ag *
 Cd 3.2
 Co *
 Cr 44
 Cu 10
 Mn 70
 Mo 10
 Ni 48
 Pb *
 Sr 200
 V 35
 Zn 19

ORGANICS

Organic C (%) 0.684
 Extractable organics (ppm) 2120
 R_o (average) 0.68

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 89.46
 H 5.64
 O 3.21
 N 1.69
 S 0.00

Atomic H/C 0.751
 O/C 0.0269
 N/C 0.0161
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 1.8x10¹⁹
 g-value Narrow -
 Broad 2.00306
 width (mT) Narrow -
 Broad 0.62

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -15.1
 Extractable organics +12.3
 Pyrite -9.5 (machine unstable)

COMMENTS

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 25

Sample number: K-13
 Stratigraphic unit: M.Devonian, U. Elk Point Gp., Watt Mountain Fm.
 Gilwood Ss.
 Well name: IOE Mitsue 4-4G1-73-4
 Location: 4-4-73-4-W5M Depth (m): 1621.5-1623.4
 Description: -
 Depositional environment: near-shore, deltaic

MAJOR OXIDES (%)

SiO₂ 32
 TiO₂ 0.3
 Al₂O₃ 12
 ΣFe as Fe₂O₃ 3.0
 MgO 1.7
 CaO 2.2
 Na₂O 0.3
 Σ 51.5

TRACE ELEMENTS (ppm)

Ag 2.1
 Cd 1.1
 Co 16
 Cr 88
 Cu 10
 Mn 68
 Mo 12
 Ni 350
 Pb *
 Sr 101
 V 97
 Zn 69

ORGANICS

Organic C (%) 0.208

Extractable

organics (ppm) 184

R_o (average) -

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C 85.08
 H 5.24
 O 6.06
 N 2.61
 S 1.01

Atomic H/C 0.734
 O/C 0.0535
 N/C 0.0262
 S/C 0.0044

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 9.1x10¹⁸
 g-value Narrow -
 Broad 2.00291
 width (mT) Narrow -
 Broad 0.42

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -
 Pyrite -

COMMENTS

For a description of this core see Kramers and Lerbekmo (1967). Composite sample taken over major shale bed (#262-264 of Kramers and Lerbekmo (1967))

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 26

Sample number: K-14
 Stratigraphic unit: M.Devonian, U.Elk Point Gp., Muskeg Fm.
 Well name: Banff Aquit Rainbow West 7-32-109-8
 Location: 7-32-109-8-W6M Depth (m): 1765.1-1765.4
 Description: -
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 60
 TiO₂ 0.9
 Al₂O₃ 16
 ΣFe as Fe₂O₃ 7.0
 MgO 2.3
 CaO 2.9
 Na₂O 0.1
 Σ 89.2

TRACE ELEMENTS (ppm)

Ag 0.5
 Cd 16
 Co 11
 Cr 221
 Cu 17
 Mn 85
 Mo 13
 Ni 260
 Pb *
 Sr 10
 V 51
 Zn 54

ORGANICS

Organic C (%) 0.560
 Extractable organics (ppm) 1120
 R_o (average) -

* = Below detection

- = Not determined

COMMENTS

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)

Adjusted for pyrite sulfur (% Fe x 1.1482)

C -
 H -
 O -
 N -
 S 0.0

Atomic H/C

O/C -

N/C -

S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -

Broad 2.1x10¹⁶

g-value Narrow -

Broad 2.00322

width (mT) Narrow -

Broad 0.46

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -

Extractable organics -

Pyrite -

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 27

Sample number: K-16
 Stratigraphic unit: M.Devonian, Nahanni Fm.
 Well name: Amoco Beaver B-2 6-19-K
 Location: b-19-K, 94-N-16
 Description: Depth (m): 4125.8
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 0.5
 TiO₂ 0.0
 Al₂O₃ 2.1
 ΣFe as Fe₂O₃ 0.2
 MgO 18.2
 CaO >9.2
 Na₂O 0.0
 Σ >30.2

TRACE ELEMENTS (ppm)

Ag *
 Cd 18
 Co 13
 Cr 233
 Cu 9
 Mn 144
 Mo 15
 Ni 136
 Pb *
 Sr 27
 V 6
 Zn 30

ORGANICS

Organic C (%) -
 Extractable organics (ppm) -
 R_o (average) -

* = Below detection

- = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C 89.52
 H 2.17
 O 1.96
 N 1.04
 S 5.31

Atomic H/C 0.289
 O/C 0.0164
 N/C 0.0099
 S/C 0.0222

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad 5.4x10¹⁸
 g-value Narrow -
 Broad 2.00316
 width (mT) Narrow -
 Broad 0.066

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen +5.2
 Extractable organics -
 Pyrite -

COMMENTS

Rare micrinite (?) and fusinite (R_o ~ 2.5)

GEOCHEMISTRY OF ALBERTA SHALES AND ASSOCIATED KEROGEN: DATA SHEET 28

Sample number: K-15
 Stratigraphic unit: M.Cambrian, Stephen Fm.
 Well name: Imperial Leduc No. 530
 Location: 8-17-50-26-W4M Depth (m): 2653.3-2659.4
 Description: -
 Depositional environment: marine

MAJOR OXIDES (%)

SiO₂ 62
 TiO₂ 0.9
 Al₂O₃ 26
 ΣFe as Fe₂O₃ 9.4
 MgO 3.1
 CaO 0.3
 Na₂O 0.1
 Σ 101.8

TRACE ELEMENTS (ppm)

Ag *
 Cd 19
 Co 11
 Cr 275
 Cu 60
 Mn 129
 Mo 11
 Ni 89
 Pb *
 Sr 113
 V 51
 Zn 129

ORGANICS

Organic C (%) 0.140
 Extractable organics (ppm) 117
 R_o (average) -

* = Below detection
 - = Not determined

ASSOCIATED KEROGEN

Normalized composition (SUM CHONS = 100)
 Adjusted for pyrite sulfur (% Fe x 1.1482)

C -
 H -
 O -
 N -
 S -

Atomic H/C -
 O/C -
 N/C -
 S/C -

ESR properties (in vacuo, corrected for pyrite)

spins/g Narrow -
 Broad -
 g-value Narrow -
 Broad -
 width (mT) Narrow -
 Broad -

SULFUR ISOTOPES (δ³⁴S ‰ CDM)

Kerogen -
 Extractable organics -
 Pyrite -

COMMENTS

For a description of the core from this well see Pugh (1971, Fig. 16)

APPENDIX B

**Organic Petrography and Reflectance Measurements
of Selected Alberta Shales**

(Report by INRS)

ARC 'COAL' PETROGRAPHY AND REFLECTANCE (R_0) ON ISOLATED SAMPLES

Author: INRS-Pétrole/HY/lm 01.10.76

Addressee: Alberta Research Council

Reference: Isolated samples

INTRODUCTION

Petrographic determination and reflectance measurement were performed on the organic matter of 15 isolated samples. Some difficulties were encountered due to the fact that the samples were assumed to be composed entirely of kerogen which was not the case. The problem was solved by a chloroform extraction. Technical problems related to the electronic stability of the reflectometer were solved and a new series of measures was obtained on the instrument.

RESULTS

A. ORGANIC MATTER PETROGRAPHY

Samples K-1 to K3: mainly composed of vitrinite-like matter associated with a high content of mineral matter. There are a few pyrofusinite particles with $2.00 < R_o < 3.75$. Vitrinite-like matter: rare cells structure, without anisotropy or fluorescence. Grain size of 4-20 microns.

Samples K-4 and K-5: mainly mineral matter with ~30% of organic matter composed of
± 50% vitrinite (télénite)*
± 40% (huminite-exinite?) ($R_o \approx 0.35$)
± 10% inertinite (semi-fusinite $R_o \approx 1.35$) (fusinite $2.0 < R_o < 5.0$)

*Vitrinite is brownish in transmitted light.

Sample K-6: same microlithotype as K-5 but with highest content of mineral material (clay, quartz, pyrite). Maceral grain size smaller than that of K-5 (≈ 10 -20 microns).

Sample K-11: less than 2% of vitrinite and other macerals in argillaceous matter.

Sample K-12: vitrinite-like substance with ~ 10% of micron-size disseminated mineral matter.

Sample K16: rare micrinite?? and fusinite ($R_o \approx 2.5$) in mineral matter.

Samples BH: trimacerite rich in mineral matter (pyrite and argillaceous material); <1% bituminite or exudatinitite (yellow fluorescence) after chloroform washing; maceral grain size <100 microns with an average of 20 microns. Huminite red brown in transmitted light ($0.12 < R_o < 0.30$); Pyrofusinite ($3.2 < R_o < 4.7$); Semi-fusinite ($1.1 < R_o < 1.7$).

Samples RCA: organic matter similar to samples BH

B. REFLECTANCE VALUES

The reflectance values obtained are shown on Table 1.

Table 1. Reflectance values

Sample no.	Low values	Ro average	High values	Low values	Ro average	High values	Lectures	Low values	Ro average	High values
K-1	.84	1.27	1.74	.82	1.28	1.82	50	.82	1.27	1.82
K-2	.41	.82	1.55	.51	.72	.98	65	.41	.79	1.55
K-3	.29	.70	1.37	.53	.67	.95	65	.29	.70	1.37
K-4	.61	.90	1.37	.40	.77	1.20	65	.40	.88	1.37
K-5	.33	.49	1.17	.32	.50	.78	65	.32	.50	1.17
K-6	.27	.44	.75	.23	.51	.84	20	.23	.47	.84
K-11	.23	.29	.40	.26	.35	.53	20	.23	.33	.53
K-12		.65		.46	.68	.90	20	.46	.68	.90
K-16			No vitrinite							
BH433-A	.27	.59	.96	.40	.65	.84	65	.27	.61	.96
BH431-G	.38	.70	1.03	.50	.60	.74	65	.38	.67	1.03
RCA65-1	.50	.72	.99	.41	.65	.85	65	.41	.70	.99
RCA67-1	.50	.68	.90	.50	.68	.84	65	.50	.68	.90
HE36				.36	.67	.93	50	.36	.67	.93
HE32-35				.39	.66	.96	50	.39	.66	.96
Reflectance values on telex dated 76-09-20				Reflectance values obtained after recalibration of instrument			Mean reflectance (in oil) Ro values calculated from the two preceding columns			