USGS
science for a changing world

Molecular Stratigraphy of the Devonian Domanik Formation, Timan-Pechora Basin, Russia

by Michele L. W. Tuttle,[1] Paul G. Lillis,[1] and Jerry L. Clayton[1]

Open-File Report 99-379

1999

U.S. DEPARTMENT OF THE INTERIOR
U.S. GEOLOGICAL SURVEY

[1]Denver, Colorado

Table of Contents

List of Tables

List of Figures

Page

Appendix Tables

Page

Page

Molecular stratigraphy of the Devonian Domanik Formation, Timan-Pechora Basin, Russia

by Michele L.W. Tuttle, Paul G. Lillis, and Jerry L. Clayton

Introduction

The Timan-Pechora Basin occupies 322,000 km^2 in northwest Russia (Ulmishek, 1982) (fig. 1). The Domanik Formation of Late Devonian age is considered the major source rock for the petroleum within this basin (possibly as much as 95% of the oil within the region; Ulmishek, 1988). The formation is mature throughout the basin except for parts of the southwestern margin of the basin where our study area is located.

The Domanik Formation is widespread throughout the Timan-Pechora Basin. The organic-rich nature of the formation is thought to have resulted from a productive water column and pelagic sedimentation in an anoxic marine environment. Variation in organic-carbon content has been attributed to changes in the magnitude of anoxia within the depositional basin (Ulmishek, oral commun., 1999).

The goal of our study is to characterize the variability in the organic and inorganic geochemistry of the immature Domanik source rock. This report tabulates our geochemical data. Complete profiles of inorganic chemistry and systematic Rock-eval data are tied to variations in lithofacies of the source rock. Lithofacies are further characterized with detailed organic geochemical stratigraphy, sulfur speciation and isotopy, and bulk mineralogy. The data tabulated herein are used to correlate the variability of lithofacies and geochemical data with changes in paleoenvironmental conditions at the time of deposition and early diagenesis of this important petroleum source.

Collaborators at VNIGRI (All Russia Petroleum Research Exploration Institute) in Ukhta, Russia, have provided field support, biostratigraphic control on sampling intervals, oil samples from the vicinity of our field area, and technical advice on petroleum geology and geochemistry of the basin.

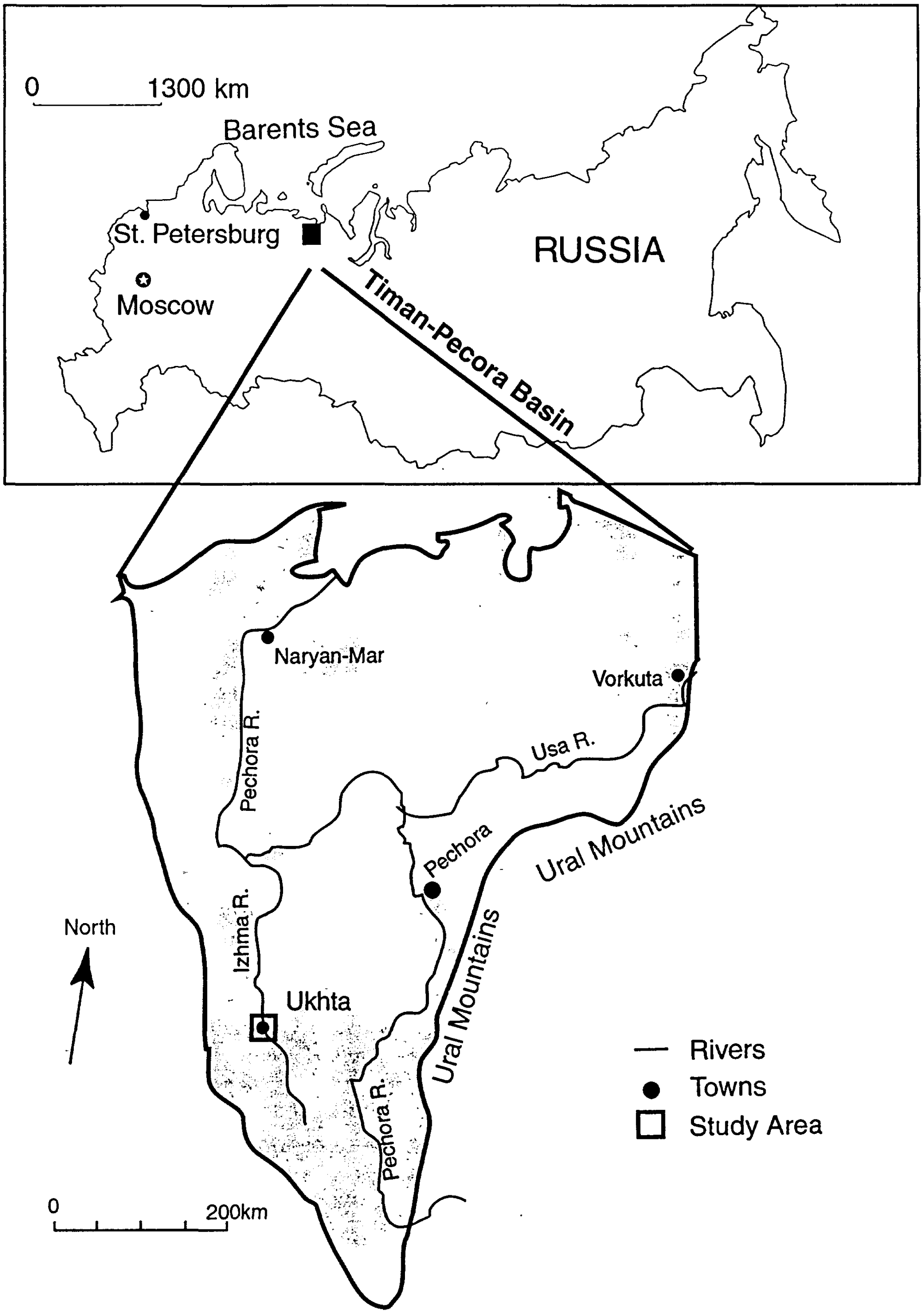


Figure 1. Index map of Russia and map of Timan-Pechora basin showing location of study area inside square around the town of Ukhta. Modified from Ulmeshek (1982).

Collaborators include Dr. Vladimir I. Bogatsky, Dr. Sergey A. Danilevsky, Dr. Yulia Yudina, and Margarita Moskalenko. Ella Bogatsky and Alexander Kutlinsky were our interpreters.

Methods

In 1995, outcrops and quarries near Ukhta, Russia, were sampled (fig. 2). The quarry locations are approximate. The sampling strategy was to collect closely spaced samples of the immature Domanik Formation. Sampling intervals in the field (fig. 3) were determined by changes in lithology, color, texture, and carbonate content as measured by reaction with hydrochloric acid. Our assumption was that changes in the depositional/diagenetic environment are reflected in the variability of these gross field characteristics.

A total of 138 samples were collected (107 in 1995 and 31 in 1994) from more than 60 meters of vertical stratigraphic thickness and tied to paleontological marker beds identified by Yudina and Moskalenko (VNIGRI, unpublished data). In addition, 13 high-resolution samples were taken in organic-matter rich intervals with a drill for Rock Eval in order to determine the scale of variability in organic matter. The stratigraphic position of the samples are given in the All source-rock samples were analyzed for total sulfur (elemental analyzer technique); total and aqua-regia extracted major-, minor-, and trace-element compositions (induction coupled plasma spectrophotometry); and organic pyrolysis characteristics (Rock-eval). The 13 drill samples were analyzed by Rock-Eval pyrolysis only. A suite of 40 samples were analyzed for whole-rock mineralogy (X-ray diffractometry) and for bulk and molecular organic composition.

The soluble organic matter was extracted by soxhlet using chloroform as a solvent. The extract was fractionated into saturated hydrocarbons, aromatic hydrocarbons, NSO compounds and asphaltenes by first precipitating asphaltenes in iso-octane followed by elution chromatography using constructed alumina/silica columns. The C_8+ saturated and aromatic hydrocarbon fractions were analyzed with a gas chromatograph (GC) equipped with a DB-1 60m x 0.32mm column and a flame ionization detector. Biomarker distributions were determined by analyzing combined saturated and aromatic hydrocarbon fractions by gas chromatography-mass spectrometry. The GC equipped with a DB-1701 60 m x 0.32 mm column was directly interfaced to a magnetic sector mass spectrometer operating in multiple ion detection mode at a mass resolution of 3000. The selected ions were m/z 191.1800 (terpanes), m/z 217.1956 (steranes), m/z 231.1174 (triaromatic steroids) and m/z 253.1956 (monoaromatic steroids). Peak identifications were based on elution time and mass spectra (Philp, 1985). Kerogen (insoluble organic matter) was isolated by digestion in HCl

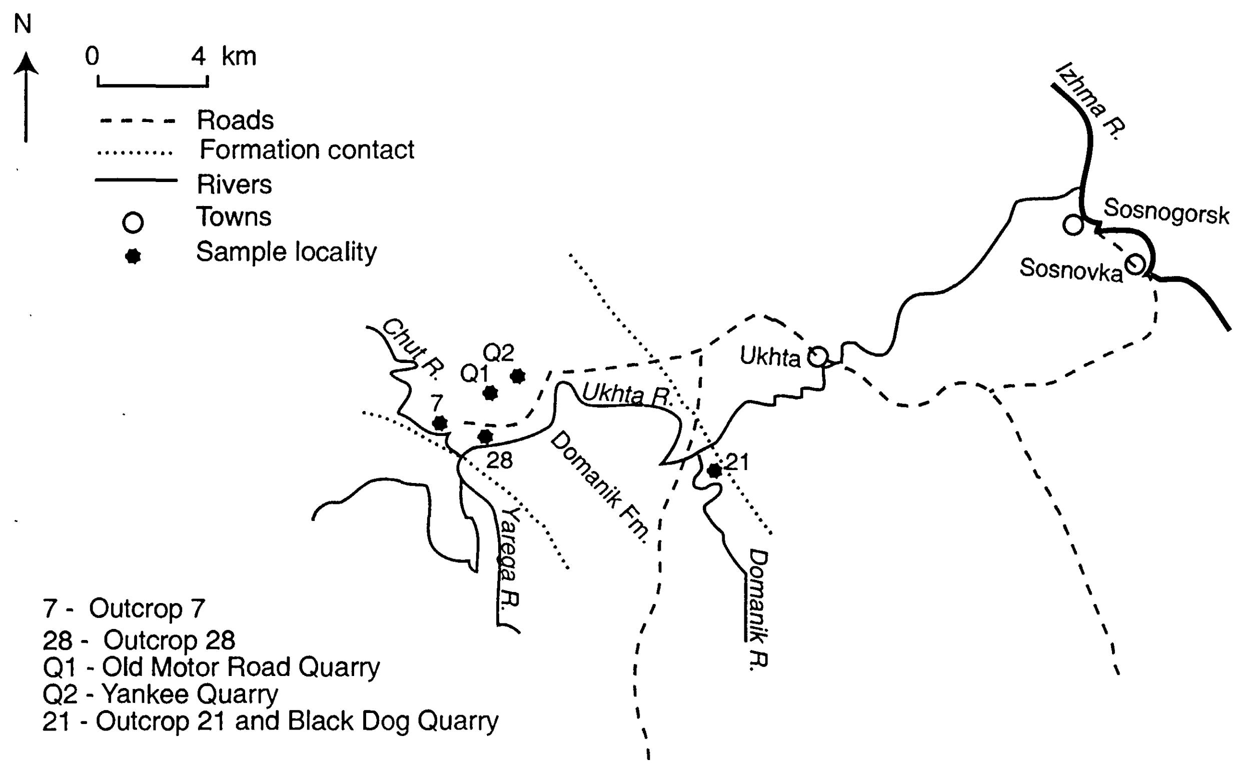


Figure 2. Domanik Formation sample localities, Ukhta area

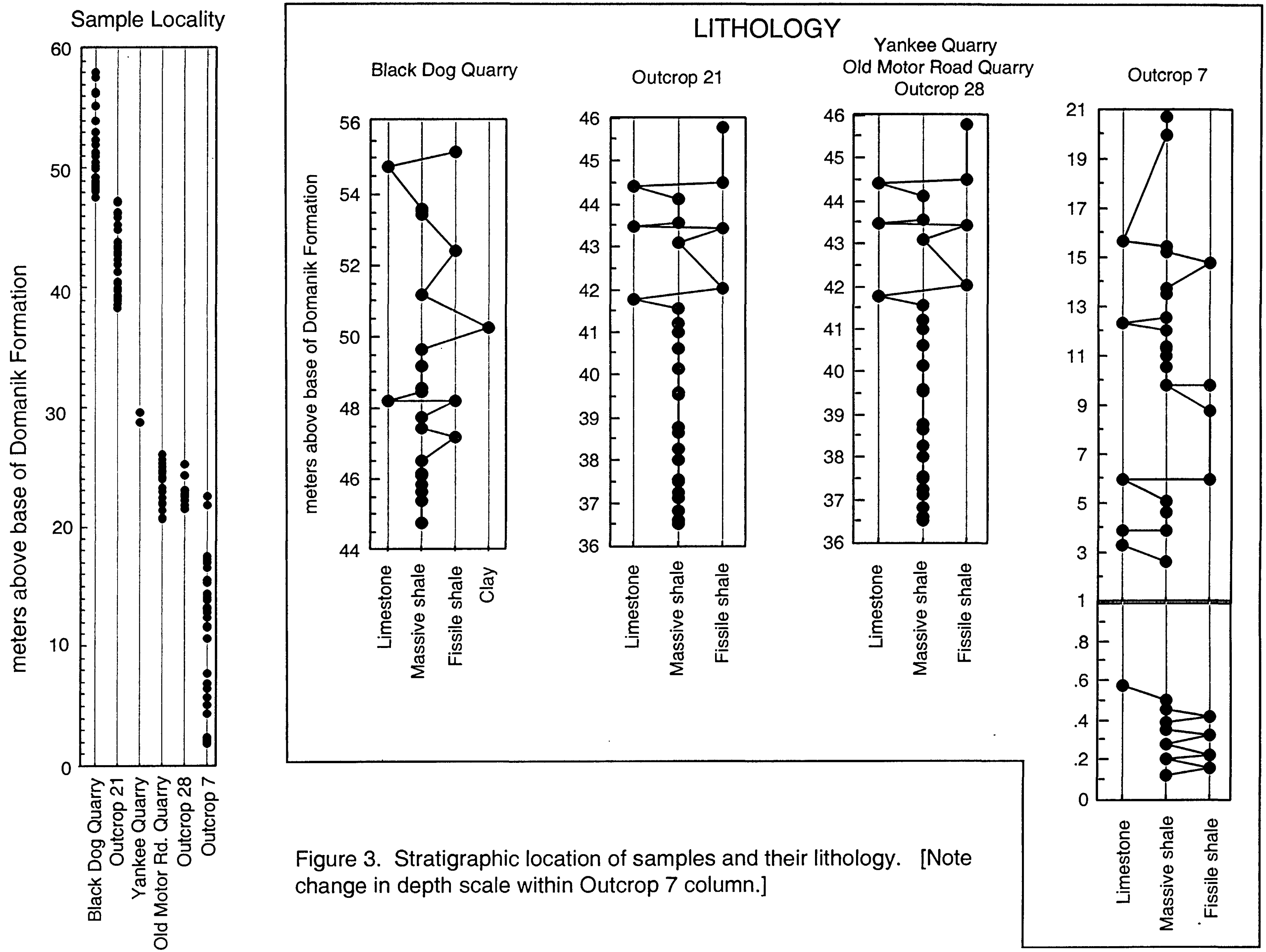


Figure 3. Stratigraphic location of samples and their lithology. [Note change in depth scale within Outcrop 7 column.]

and HF followed by separation with $ZnBr_2$. Stable carbon isotope ratios were determined for the C_{15}+ saturated and aromatic hydrocarbon fractions and the kerogen fraction by analyzing the CO_2 from sealed quartz tube combustion with a dual inlet isotope ratio mass spectrometer. The results are expressed in the delta (δ) notation that represents the deviation of the $^{13}C/^{12}C$ ratio in parts per thousand (per mil, or ‰) relative to the Peedee belemnite (PDB) standard. Isolated kerogen was analyzed for hydrogen, carbon, oxygen, and nitrogen by combustion on a CHNO elemental analyzer. Nickel and vanadyl porphyrins in the extracted bitumen were measured with a ultraviolet/visible diode array spectrophotometer. Analytical results are tabulated in the Appendix.

The suite of 40 samples plus 34 others were analyzed for sulfur phases (wet-chemical separation and gravimetric determination; Tuttle and others, 1986) and for sulfur isotopic composition of each phase (Tuttle, 1988). The isotope results are expressed in the delta (δ) notation that represents the deviation of the $^{34}S/^{32}S$ ratio in parts per thousand (per mil, or ‰) relative to the Cañon Diablo Troilite (CTD) standard. Analytical results are tabulated in the Appendix. Thin sections were prepared from 19 representative samples and examined by transmitted- and reflective-light microscopy.

Included in Appendix tables A1 and A2 are estimates of various mineral phases calculated from chemical data. The amount of calcite (the only carbonate phase identified with X-ray diffraction) was calculated with the formula below:

$$\text{calcite \%} = (\text{Ca\% (AR)} * 1.25) + (\text{Mg\% (AR)} * 3.5).$$

We assume that all calcium and magnesium extracted in the aqua-regia treatment resided in this carbonate phase. Clay content was calculated assuming all aluminum resides in illitic or kaolinitic clays (assumptions are substantiated with X-ray diffraction data and transmitted-light microscopy):

$$\text{clay \%} = \text{total Al\%} * 4.8.$$

Silica (SiO_2 as quartz) was calculated from the following equation:

$$SiO_2\ \% = 100 - ((\text{organic C \%} * 1.25) + \text{clay \%} + \text{calcite \%})),$$

where (organic C % * 1.25) is organic carbon content converted to percent organic matter. The calculated SiO_2 values correlate very well with quartz peak heights from the X-ray diffractograms.

The Geochemistry of Domanik Source Rocks

Lithology and Mineralogy

The Domanik source rocks contain predominantly quartz, calcite, and varying amounts of organic matter and clay (fig 4). With the exception of two samples, clay contents are anomalously low, almost always less than 10 wt% even in most fissile shaly samples (figs. 4 and 5). Conversely, calculated SiO_2 contents are high, nearly 100 wt% in end-member samples (right side of fig. 4A). The dominant SiO_2 phase is by far quartz (fig. 5). Detrital quartz is ruled out as the dominant source because other detrital minerals associated with clastic sediment are very minor, and no evidence of eolian sand grains was observed in thin sections. The origin of most the quartz must be biogenic opal that recrystalized to fine-grained quartz with increasing temperature. Thin sections do show silicified remains of organisms in samples containing large SiO_2 contents. The other end member on figure 4A is also a biogenic component--calcite that forms limestone--defined here as sample having greater than 50 wt% calcite (Bates and Jackson, 1980). The limestone is composed of variable amounts of calcite and silica (<40%) with very small amounts of clay or organic carbon.

Organic Geochemistry

The amount of organic carbon in the rock is controlled by dilution with minerals, primarily biogenic SiO_2, and, secondarily, calcite and clay in the sample (fig. 4), The highest organic contents are in fissile shale. Despite the wide variability in lithology and organic-carbon content, the gross organic facies type is remarkably uniform as indicated by the narrow range in H/C composition (1.10-1.24). For example, the lowest portion of the Domanik has an organic-carbon range of 0.8 to over 25 weight percent while the H/C ranges only from 1.13 to 1.21 (fig. 6). This would classify the organic matter as Type II kerogen as defined by Tissot and others (1974). Furthermore, there is a good correlation ($r = .98$) between the pyrolysis S_2 values (generated hydrocarbons/gm organic carbon) and organic-carbon values (fig. 7). The "true" average Hydrogen Index (HI) is the slope of the regression line for this correlation (Langford and Blanc-Valleron, 1990), which is equal to 553 mg HC/g organic carbon. Because of the similarity in the type of organic matter within the section, the amount of oil that can be generated from the rock (generative potential) is only dependent on the amount of organic carbon in the rock (fig. 7). All but the limestones have very good generative potential (Peters, 1986). The HI versus Oxygen Index (OI) plot (fig. 8) relate sample data to Types I, II and III kerogen maturation curves (Espitalie and others, 1977).

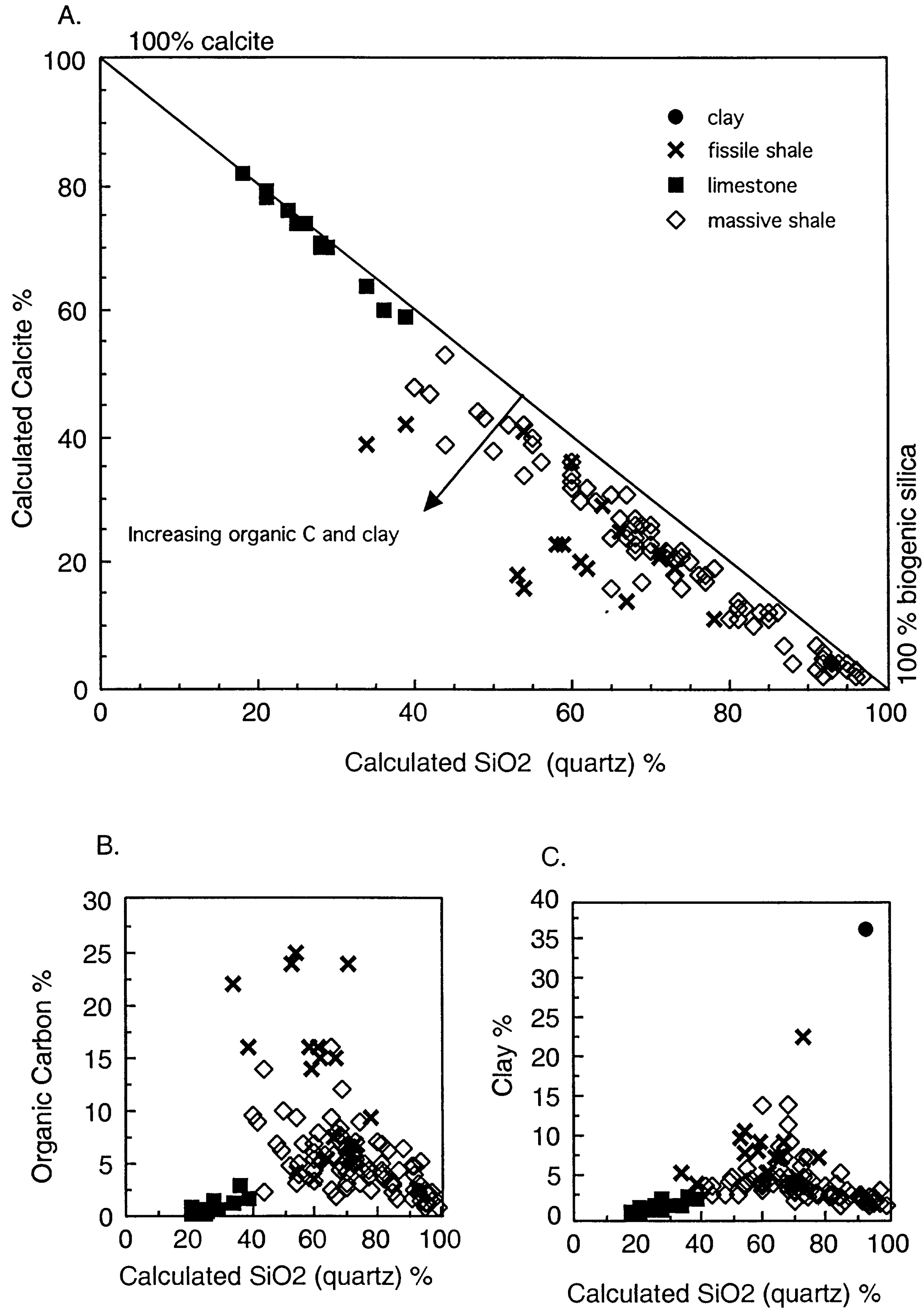


Figure 4. Crossplots of (A) calculated calcite (wt%), (B) organic carbon (wt %), and (C) calculated clay (wt %) versus calculated silica (quartz) (wt %).

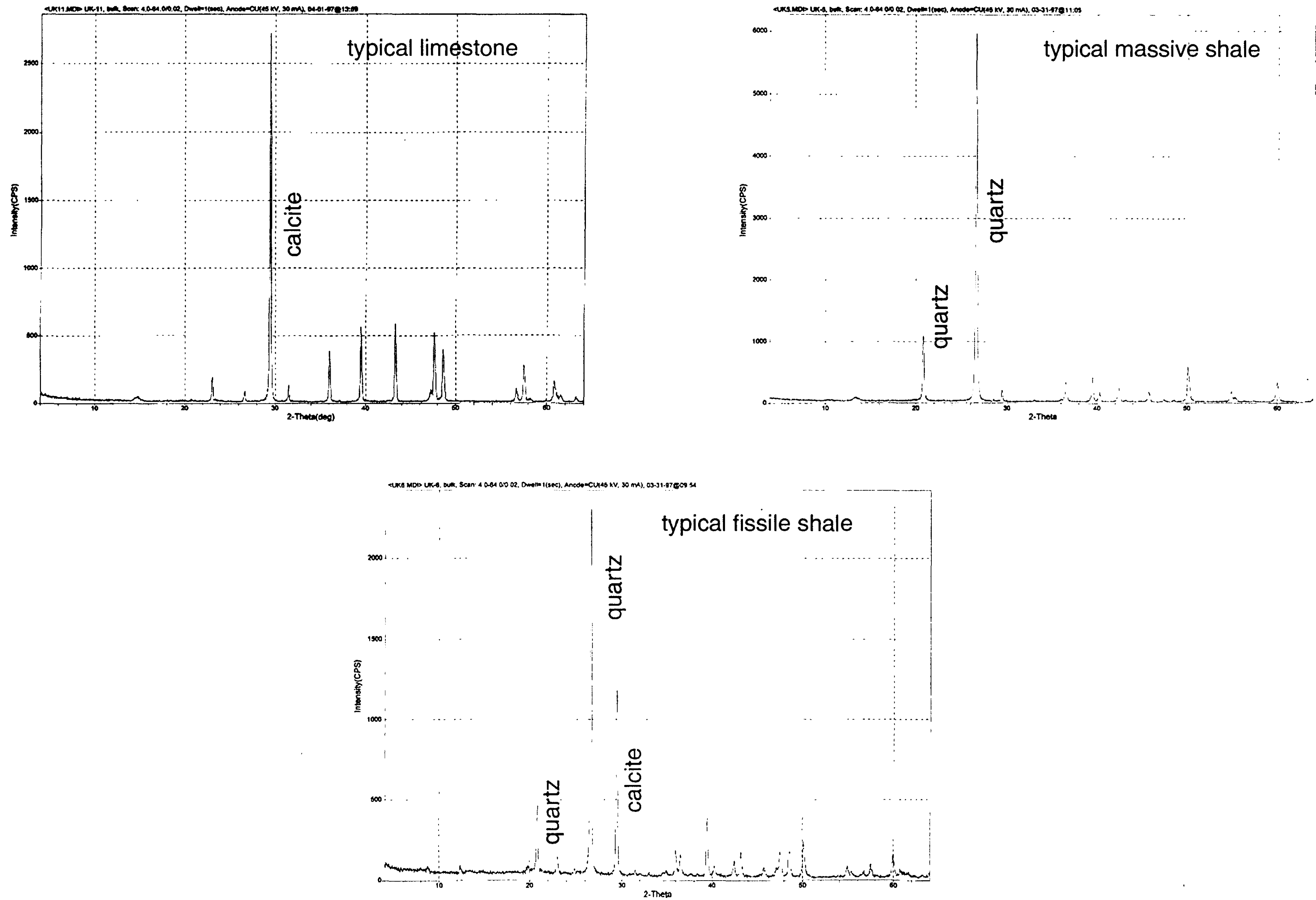


Figure 5. X-Ray diffraction traces of a typical limestone, massive shale, and fissile shale from the Domanik Formation.

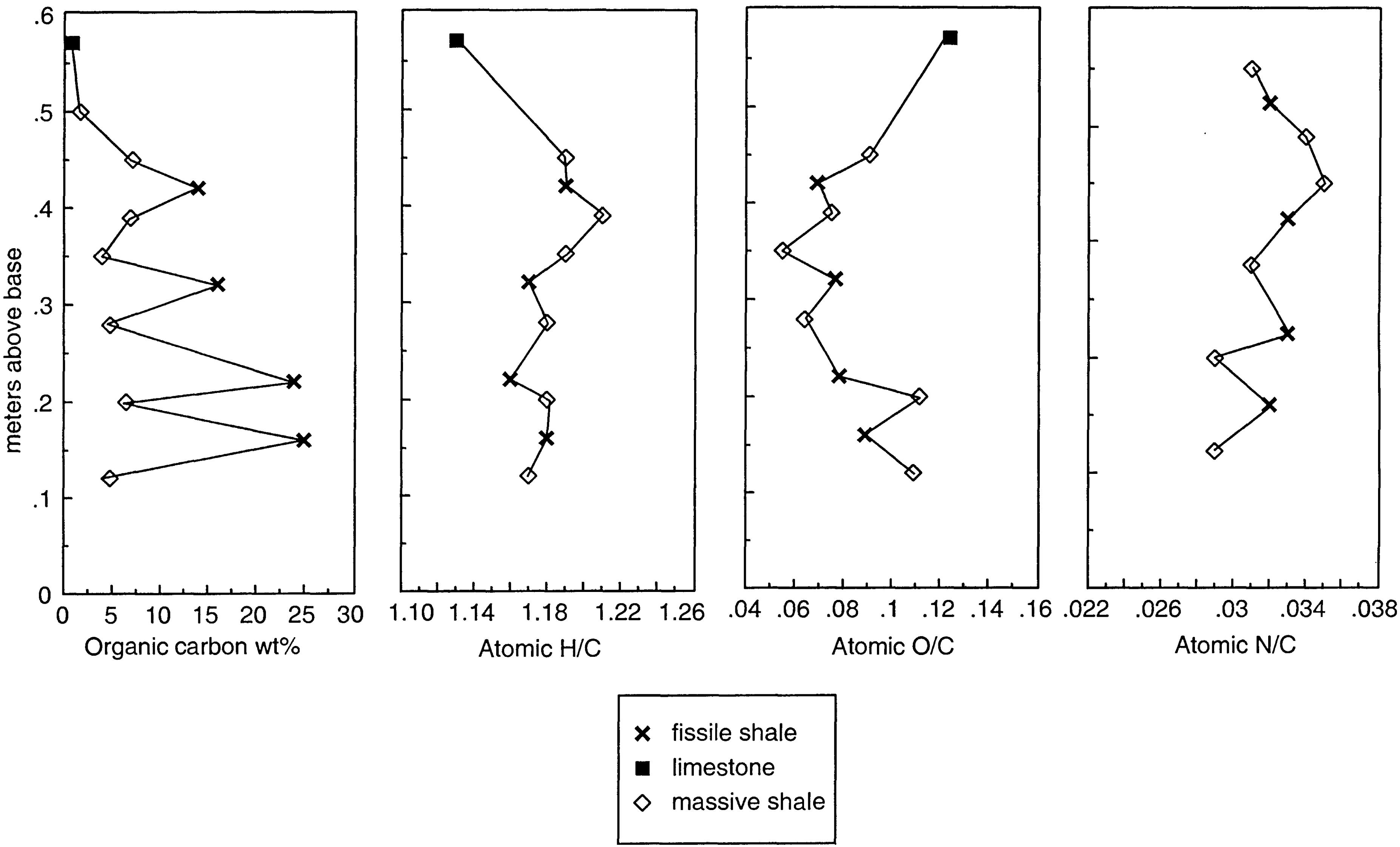
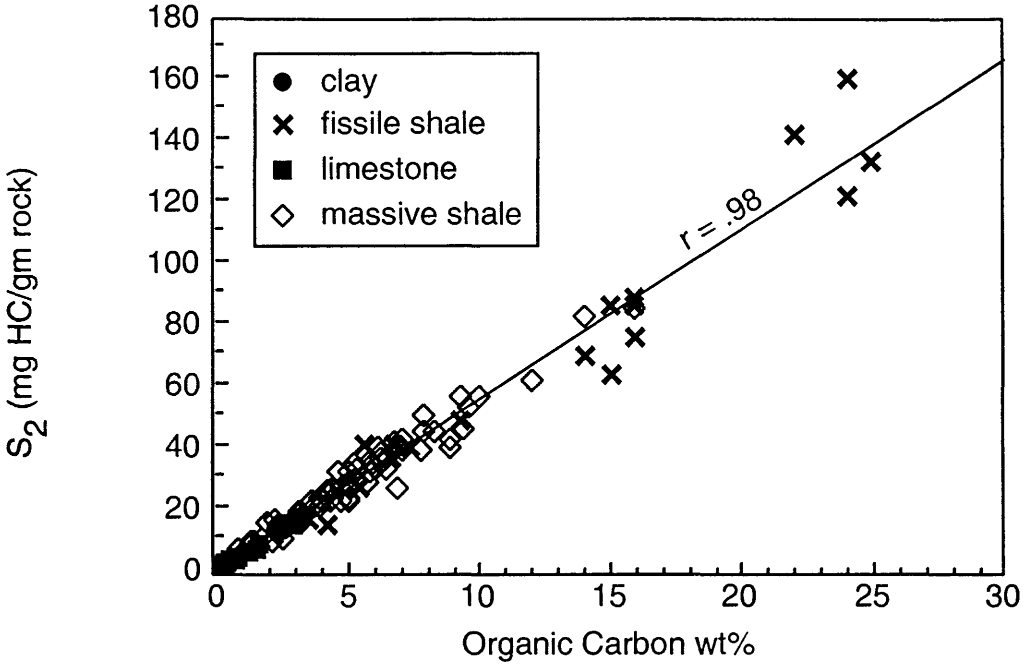


Figure 6. Organic carbon content and kerogen elemental composition from the lower 0.6 meters of the Domanik Formation.



S_2 mg/g = .656 +5.5Organic Carbon wt%

Figure 7. Crossplot of S_2 (mg HC/gm rock) versus organic carbon (wt%).

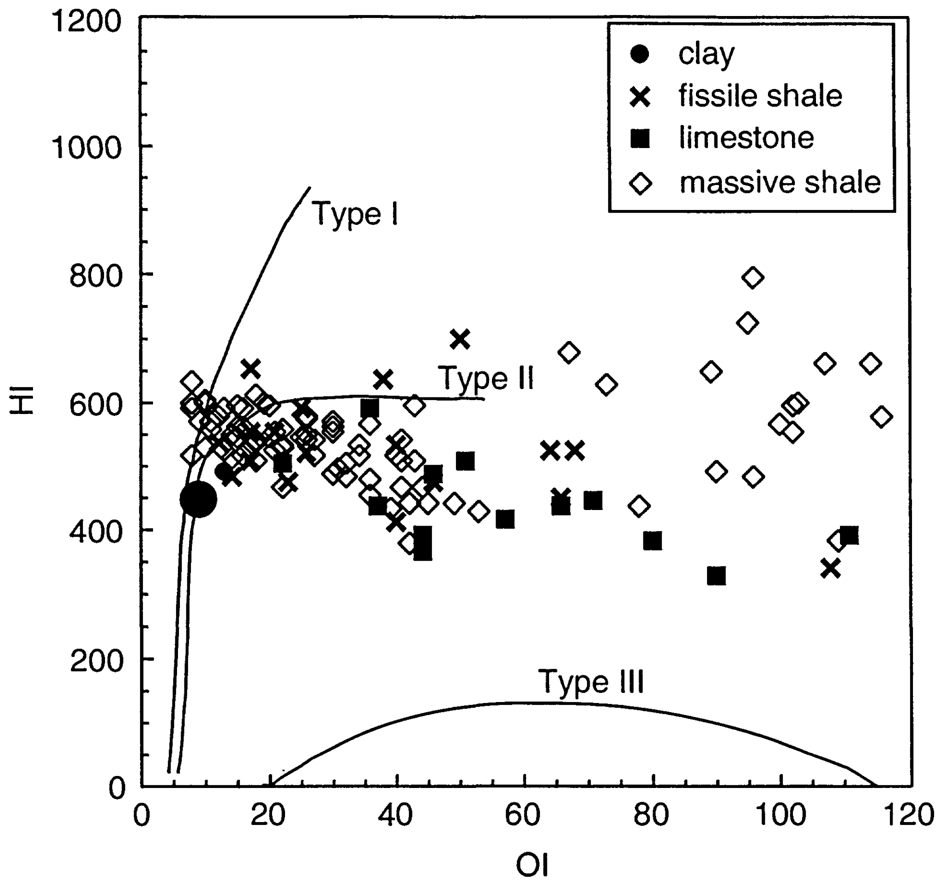


Figure 8. Crossplot of HI versus OI.

Samples with OI values greater than 60 on the average have the same carbonate content as those with values less than 60.

The extractable organic matter/organic carbon (EOM/organic carbon) ratios are variable depending on the lithology and are, on average 22% (table A5; fig. 9), unusually high for immature source rocks. Domanik Rock-Eval T_{max} values are generally less than 430°C while the beginning of the typical oil window is approximately 435°C and peak oil generation is approximately 445°C (Peters, 1986). In immature source rocks, EOM/organic-carbon ratios greater than 20% are often attributed to non-indigenous hydrocarbons that have migrated from mature sources elsewhere (Hunt, 1979, p. 267; Tissot and Welte, 1984, p 514). However, there are many examples of immature clay-poor source rocks such as the Austin Chalk, and rocks in the Los Angeles and Ventura Basins that have high amounts of indigenous bitumen and EOM/organic-carbon values exceeding 20% (Hunt and McNichol, 1984; Leigh Price, written commun., 1999). Because the Domanik is clay-poor and because the average S_1:organic-carbon ratio (0.7) is significantly less than 1.5 (Hunt, 1996, p. 491), the extractable organic matter is interpreted as being indigenous. The high EOM/organic carbon ratios are due to either early bitumen/oil generation from thermal maturation or reduced polymerization of organic matter due to extremely reducing conditions during diagenesis (Powell, 1984).

The $\delta^{13}C$ kerogen values show a negative shift in the first few meters above the base of the Domanik, and a large positive excursion at 50.25 meters above the base of the Domanik (sample 96018-089) which is in the Middle to Upper Domanik (fig. 10). The isotopic shift observed at about 20 meters above the base of the formation may be caused by differences in outcrop locality. The lower ten samples show an approximately one per mil variation in the $\delta^{13}C$ aromatic hydrocarbon values which correspond with the total organic carbon content and lithologic variations observed in the field (figs. 3, 6, 10). However, the $\delta^{13}C$ kerogen values show minimal variation in this same interval. The $\delta^{13}C$ saturated hydrocarbon values are relatively uniform throughout the Domanik (fig. 10).

Vanadium- and nickel-pophyrin concentrations in the bitumen are high relative to those in bitumen from other source rocks (Lewan and Maynard, 1982); values range from 67 to 6633 ppm V porphrin and 15 to 1814 ppm Ni porphyrin (fig. 11).

The overall biomarker compositions of the bitumen extracts are quite consistent throughout the Domanik Formation with some minor variations of the tricyclic, pentacyclic terpanes. The lowest sample (96018-001) and the highest sample (96018-094) are nearly identical in biomarker composition (table A7)

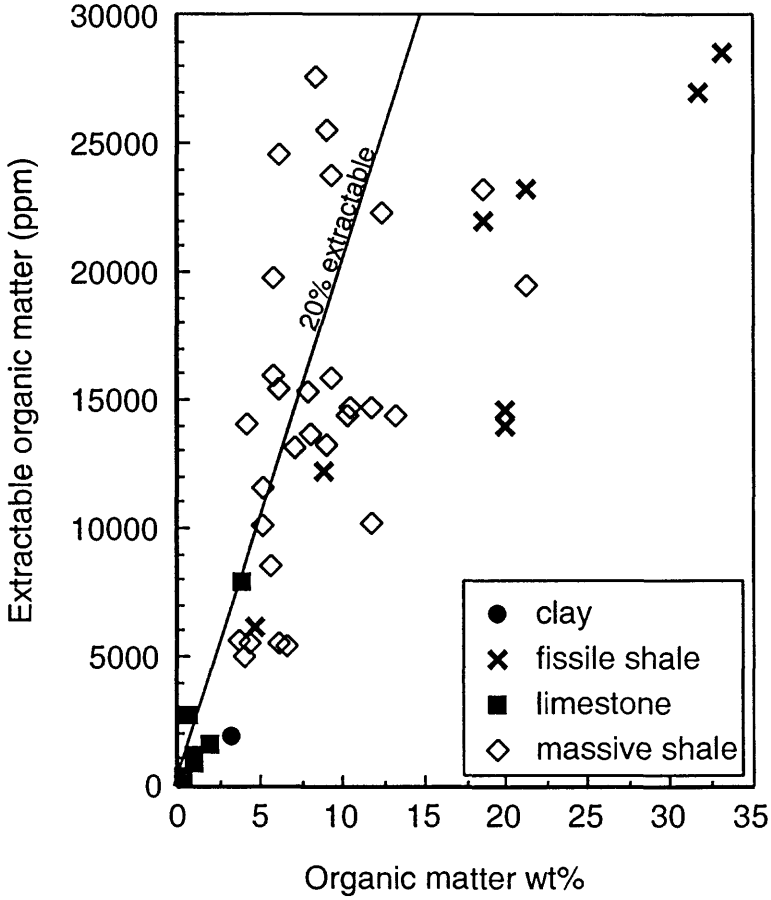


Figure 9. Crossplot of extractabable organic matter versus total organic matter. Organic matter was calculated using 1.326 times the organic carbon value. This conversion factor was derived from atomic composition of the organic matter and was constant throughout the data set.

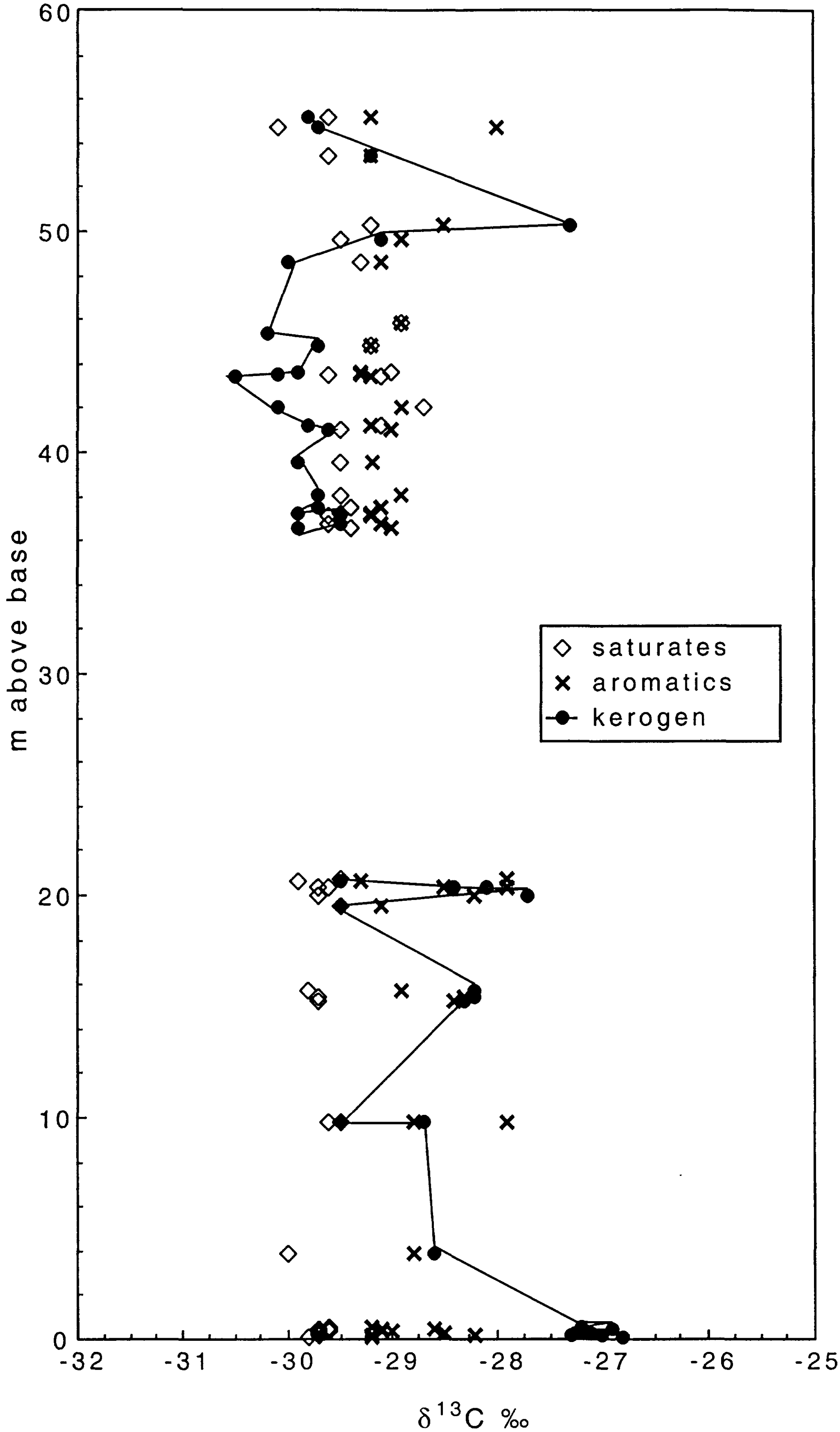
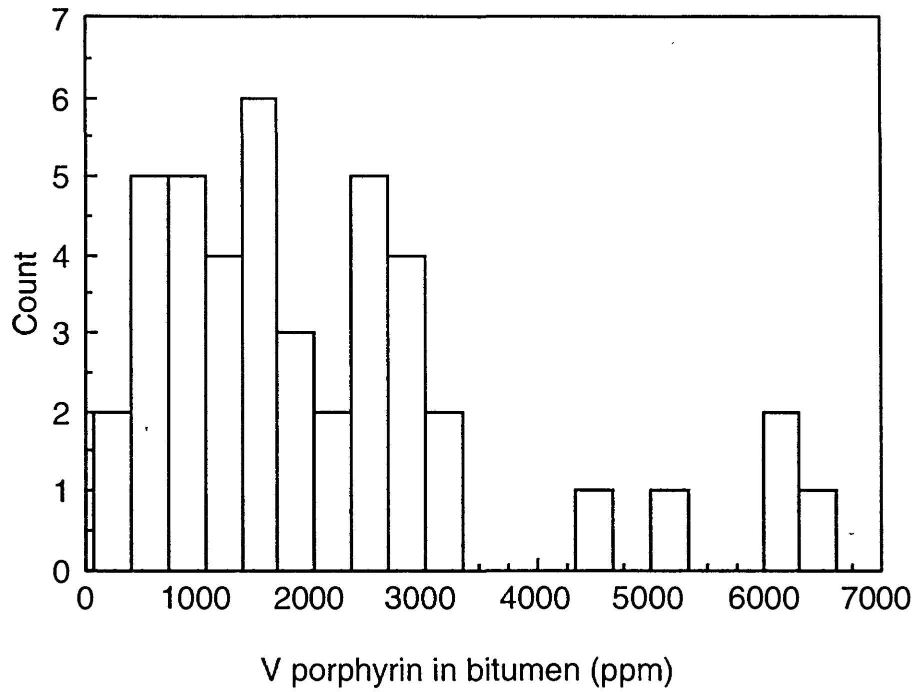


Figure 10. Stable carbon isotope values of the kerogen fraction and the saturated and aromatic hydrocarbon fractions of the Domanik Formation.

A.



B.

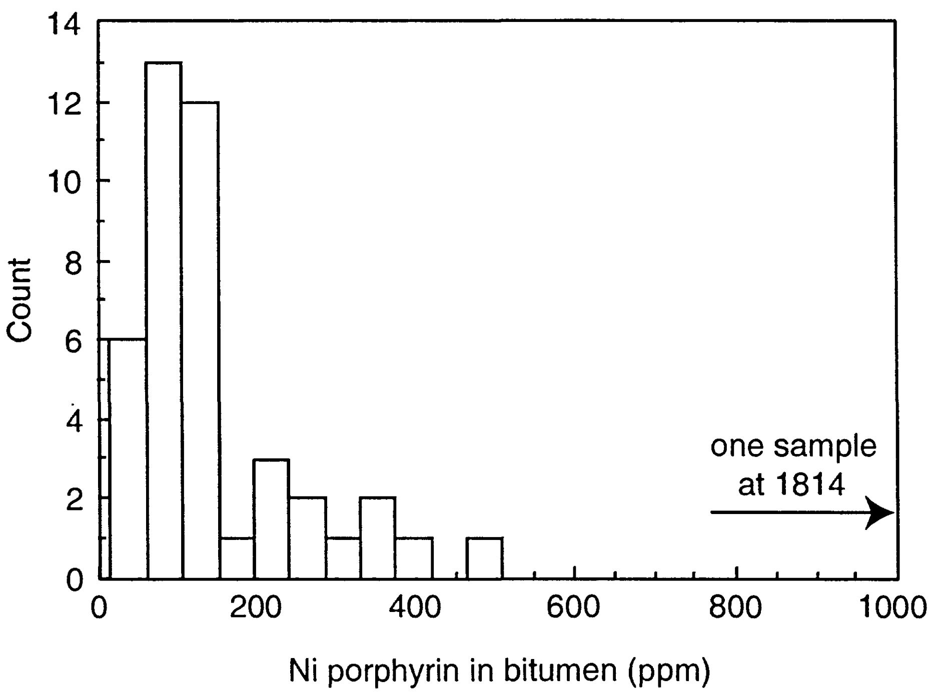


Figure 11. Histograms of (A) V porphyrin (ppm) and (B) Ni pophyrin (ppm) in bitumen.

despite the three per mil difference in the $\delta^{13}C$ kerogen values.

In general, the Domanik tricyclic/pentacyclic terpane mass chromatograms (m/z 191) look quite typical with dominant C_{30} hopane and secondary norhopane, and decreasing concentrations of the C_{31} to C_{34} homohopanoids with a slightly elevated C_{35}. The Ts/Tm values range from about 0.4 to 0.6, the C_{23} tricyclic terpane/hopane values range from about 0.2 to 0.4, and the C_{24} tetracyclic terpane is approximately the same concentration as the C_{26} tricyclic terpane isomers. Gammacerane/hopane values are normal (0.05 to 0.15) except for samples 96018-036, 96018-037 and 96018-093 which have elevated values (>0.3).

In general, the Domanik sterane mass chromatograms (m/z 217) show low concentrations of diasteranes and pregnanes, and the C_{29} steranes are slightly greater than C_{27} steranes noticeably larger than C_{28} steranes. Small C_{30} and C_{26} steranes are recognized but are minor.

The dramatic sawtooth pattern observed in the TOC and $\delta^{13}C$ aromatic hydrocarbon data for the Lower Domanik is not reflected significantly in the biomarkers. An exception is seen in the relative percentage of C_{27} steranes and tricyclic terpanes, and to a lesser degree the biomarker maturity parameters such as C_{31} S/S+R (see example in fig. 12).

The Domanik Formation is slightly more thermally mature to the east (Outcrop 21) than to the west (Outcrop 7 or 28) based on a number of biomarker maturity parameters, including S/S+R C_{29} steranes (C29SR), $\beta\beta/\beta\beta+\alpha\alpha$ C_{29} steranes (C29BBAA), triaromatic cracking (TRIOCR), Ts/Tm, moretane/hopane (MOR/HOP), and the C_{29} neonorhopane/norhopane (NEO/NOR) ratios. For example, the S/S+R C_{29} sterane (C29SR) values of the western outcrop average 0.32 whereas the eastern outcrop values average 0.38. However, the difference in thermal maturity between west and east is not apparent based on Rock-Eval Tmax, S/S+R C_{31} hopanes (C31HSR) or triaromatic/monoaromatic sterane (T/T+M) values.

Trace Metal Geochemistry

Most metal contents in the Domanik Formation are positively correlated with organic-matter contents. The total concentration of metals such as Ni, Cu, Zn, Mo are essentially the same as respective concentrations in the aqua-regia extractions (1:1 correlation with r values of .95 to .99; fig. 13). The extractable metals are primarily associated with organic carbon and perhaps, secondarily, with oxy-hydroxides, both of which are decomposed by aqua-regia. Total vanadium concentrations are twice that measured from

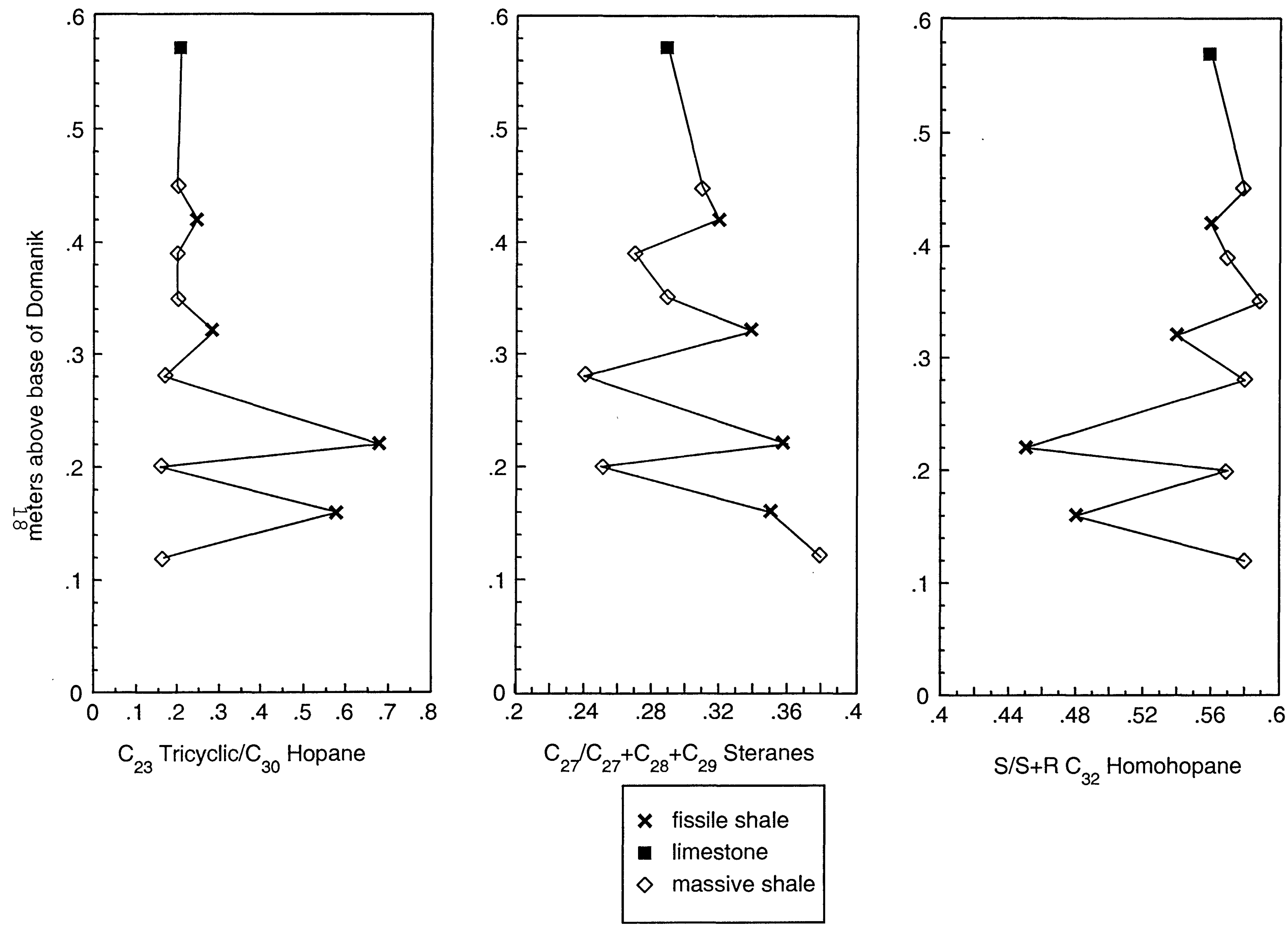


Figure 12. Extract biomarker composition of the lower 0.6 meter of the Domanik Formation.

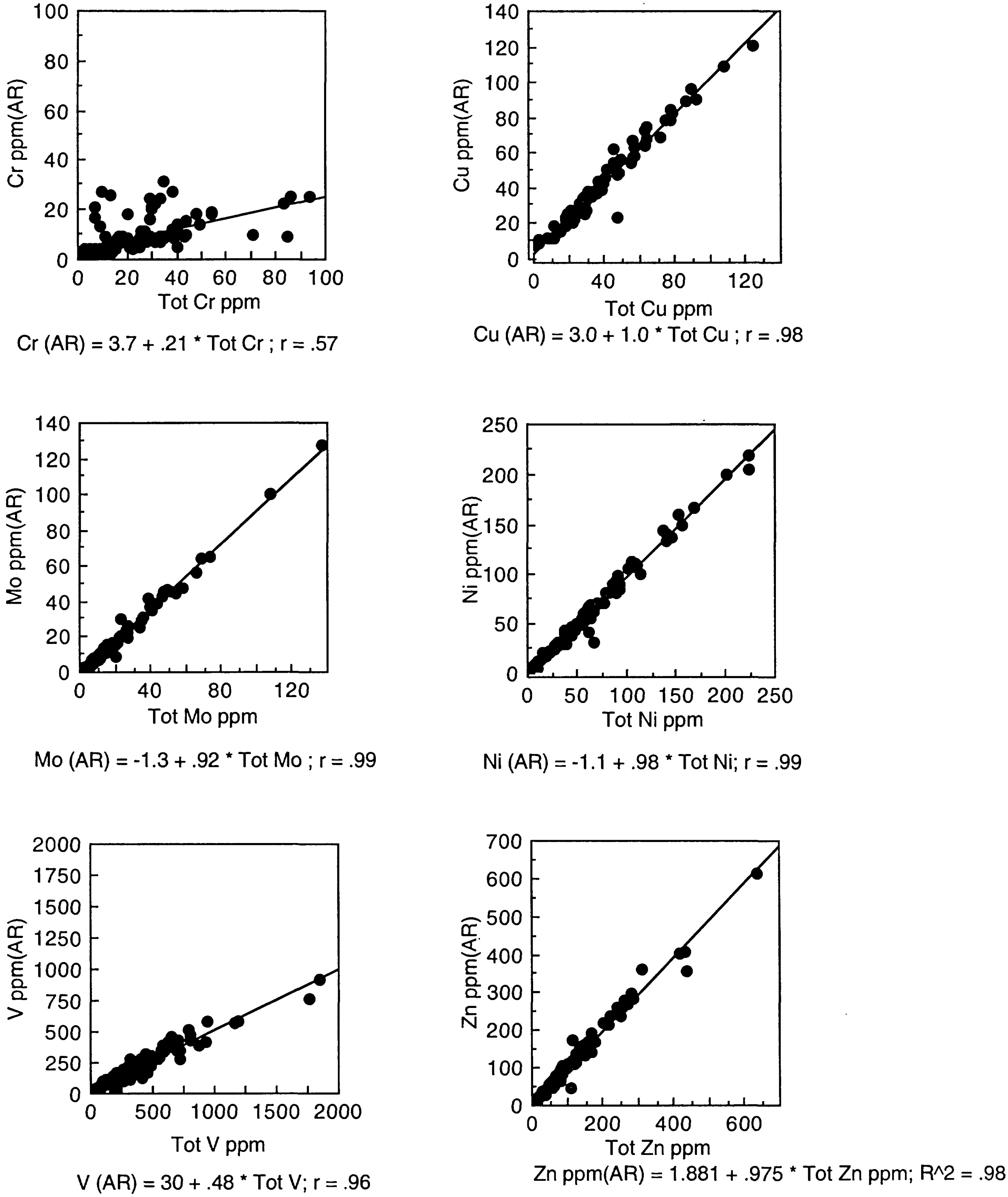


Figure 13. Crossplots of metal concentrations in aqua-regia extracts (AR) versus bulk rock (Tot).

the aqua-regia extraction, but the two concentrations are highly correlated (r value of 0.93). Total chromium is, on the average, five times greater than aqua-regia extractable chromium, with the two values not correlated. Half the vanadium and the majority of chromium are associated with resistate minerals that are not solubilized by aqua-regia. In the case of vanadium, the mineral is associated with the organic matter to preserve the high correlation between the total and extractable concentration; clay is the most probable mineral.

Metal enrichment is dependent on redox conditions during deposition and on metal source. If the metal source is sea water, then metal accumulation also is controlled by the amount of time that the sediment remains "open" to metal-bearing waters. The degree of "openness" is sensitive to such factors as watercolumn turnover rates, sediment accumulation rates, and porosity of the sediment (Lewan and Maynard, 1982). To separate the influence of redox conditions from metal supply, metal ratios, such as V:(V+Ni) ratio, are often used because different metals preferentally accumulate under different redox conditions (Lewan, 1984).

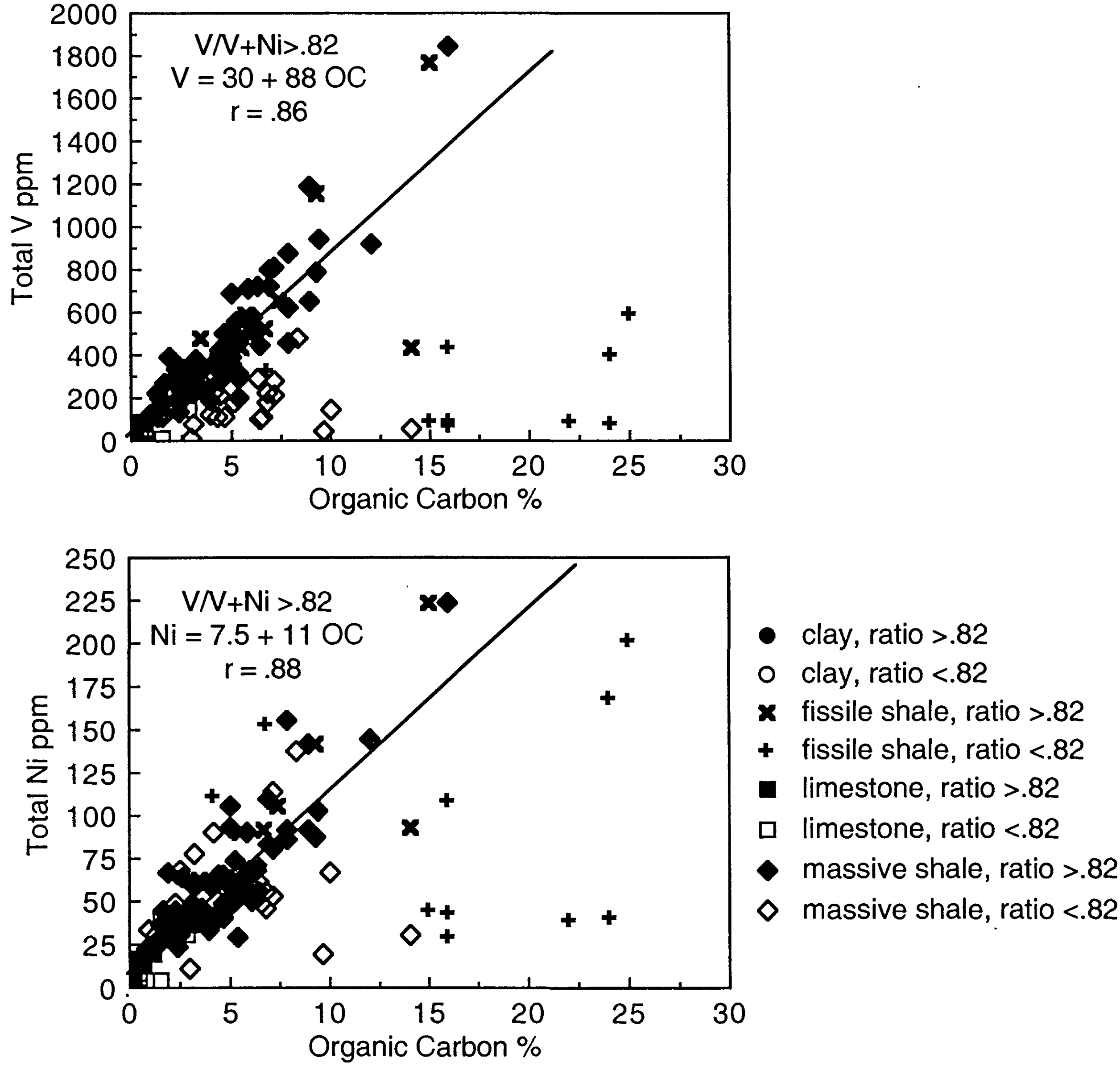
The V:(V+Ni) ratios in the Domanik (average of .82) are consistent with an anoxic to euxinic (H_2S-bearing) bottom waters (Hatch and Leventhal, 1992). Metal contents, although high relative to average shale abundance, are less than those in some marine shales deposited under similar euxinic conditions (i.e. similar V:(V+Ni) ratios) (table 1). The lower metal contents suggest that the sediment accumulation rates were greater than in the "metalliferous" shale, isolating the sediment more quickly from the overlying water column, thus inhibiting accumulation of metals over time. Additionally, fissile shale has metal contents that, on the average, are much lower than expected from their organic-carbon content (fig. 14). Accumulation of the fissile shale was more rapid than accumulation of the massive shale. In support of this hypothesis, the fissile nature of the shale cannot be attributed to high clay contents, and may have resulted from rapid accumulation of layers of organic matter. Such layers form in mineral-poor turbidite sequences (see Dean and others, 1984 for discussion on the role of turbidites in formation of Cretaceous black shale in the Atlantic).

Unlike most metal contents, that of iron is not related to organic-carbon, and is low with an average of 0.46 wt % compared to 4.7 wt % in the average shale (Krauskopf, 1979). The low contents are due to low content of detrital minerals in the shales. On the average, 25 % of the iron in the sediment resides as pyrite.

Table 1. Selected trace element concentrations and V:(V+Ni) ratios in a variety of shales and sediments.

Shale/Sediment	Cr ppm	Cu ppm	Mo ppm	Ni ppm	V ppm	Zn ppm	V/(V+N)	References
Average shale	100	50	2	140	130	80	0.48*	tabulated in Krauskopf '79
Modern Oxidized Pelagic clay	90	250	27	225	120	165	0.35*	Chester and Aston'76 as cited in Dean '84
Modern Baltic Sea Sediment/anoxic	90	78	35	43	130	110	0.75*	Manheim '61 as cited in Dean '84
Modern Black Sea Sediment/euxinic	143	38	13	82	225	98	0.73*	Hirst '74 as cited in Dean '84
Cretaceous Black Shale-Angola Basin	222	170	26	181	692	782	0.78*	Dean '84
Devonian Domanik Fissile Shale	34	61	33	100	470	165	0.78	This Study
Devonian Domanik Massive Shale	23	30	18	60	375	100	0.83	This Study
Pennsylvanian Stark Shale-euxinic	510	125	510	435	2520	2730	0.85	Hatch '92
Pennsylvanian Stark Shale-anoxic	465	70	210	275	1150	1290	0.72	Hatch '92
Pennsylvanian Stark Shale-euxinic/anoxic	480	90	315	330	1630	1800	0.77	Hatch '92

*Calculated using average V and Ni concentrations



- ● clay, V/V+Ni ratio >.82
- ○ clay, V/V+Ni ratio <.82
- ✖ fissile shale, V/V+Ni ratio >.82
- + fissile shale, V/V+Ni ratio <.82
- ■ limestone, V/V+Ni ratio >.82
- □ limestone, V/V+Ni ratio <.82
- ◆ massive shale, V/V+Ni ratio >.82
- ◇ massive shale, V/V+Ni ratio <.82

Correlation Coefficient for samples with V/V+Ni >.82	
Mo	r = .69
Cu	r = .88
Zn	r = .72
Cr	r = .77
P	r = .81

Figure 14. Crossplots of total vanadium and total nickel (both in ppm versus organic carbon (wt%), with correlation coefficients for other metals.

Pyrite formation undoubtedly was limited by the amount of reactive iron available during production of H_2S by sulfate-reducing bacteria in the sediment. Pyritic sulfur in the Domanik source rock is enriched in ^{34}S ($\delta^{34}S$ values between 2.6‰ and 21.0‰) when compared to most marine shales ($\delta^{34}S$ commonly near -20‰). A similar enrichment is reported for pyrite in Monterey Formation source rock ($\delta^{34}S$ values between -18‰ and 11.9‰; Zaback and Pratt, 1992). Isotopic compositions of organosulfur in both formations are similarly enriched (1.8‰ to 21.7‰ in the Monterey; Zaback and Pratt, 1992, and 8.9 to 22.5‰ in the Domanik; this study). Zaback and Pratt (1992) attribute the ^{34}S-enrichment in organosulfur relative to pyrite in the Monterey to (1) formation of pyrite at the sediment/water interface under mildly reducing conditions and (2) formation of organosulfur deeper in the sediment when strongly reducing conditions were established. The more ^{34}S-enriched isotopic values in the Domanik pyrite suggest near complete reduction of sulfate by bacteria and pyrite formation in the same zone as organosulfur. As discussed earlier, high V:(V+Ni) and EOM:organic carbon ratios in the Domanik are consistent with highly reducing, likely euxinic bottom waters. In modern euxinic oceans/seas, the $\delta^{34}S$ value of the H_2S in bottomwater layers is far more depleted in ^{34}S than sulfur in Domanik pyrite ($\delta^{34}S$ values average +12‰). For example, $\delta^{34}S$ values of H_2S in the bottom water of the Black Sea are -36‰ to -41‰ (Fry and others 1991) and in Framvaren Fjord, Norway, values are between -22‰ and -11‰ (Sælen and others, 1993). If the Domanik was deposited in euxinic water, then one of two scenarios is required. First, the bottomwater layer had to be extremely stable with respect to mixing and most of the sulfate bacteriogenically reduced, increasing the $\delta^{34}S$ of the H_2S. Alternatively, the bottom water could have been euxinic and rapid accumulation rates resulted in isolating pore water where additional bacterial activity reduced most of the remaining sulfate. This latter scenario explains, in part, the ^{34}S-enrichment in pyrite in relatively shallow sediment of the Black Sea (albiet the enrichment is smaller than in the Domanik). Either scenario supports the lower metal contents observed in the Domanik shales relative to sediment deposited in an euxinic, but less restricted water or sediment column.

Because the amount of iron available for pyrite formation was low, excess H_2S reacted with organic matter. The $S_{organic}/C_{organic}$ ratios average 0.03 compared to ratios of 0.01 in living organisms. Twenty percent of the values are greater than 0.04, a value above which source rocks generate sulfur-rich oils at lower temperatures than estimated for most source rocks (Orr, 1986).

Paleoenvironmental Conditions during Deposition of the Domanik Formation

The Domanik Formation was deposited in an euxinic marine basin during the highest sea level rise of the Late Devonian Epoch. Water depths were sufficiently deep to preserve laminated sediments and isolate euxinic bottomwater layers from frequent mixing. This deepwater-restricted deposition was periodically interrupted. The deepwater shales are massive to fissile silicieous pelagic rocks composed of biogenic silica, with varying amounts of clay and calcite. The extremely low clay content and the lack of other clastic minerals in these shales indicate a long distance to the nearest strandline, or a basin isolated by landward banktops/sills and adjacent proximal basins.

The organic matter deposited is remarkably uniform with respect to gross composition. Organic-matter concentration in the sediment was controlled primarily by dilution of biogenic silica produced in the overlying water column, which in turn was controlled by upwelling. The variation of organic carbon in figure 15 is suggestive of cycles within variable depth intervals that are more or less complete depending on sample density. The 0.5-m cycle (.12 to .57 m above base) illustrates two orders of cycles. The large cycle (0.5 m) is comprised of at least 4 smaller cycles and is bounded by two limestone beds (fig. 3), the lowermost being the basal Domanik limestone at 0 m. Limestone throughout the section generally has much lower organic carbon contents than adjacent shale (0.77 wt % organic carbon in the upper limestone bed of this cycle). Deposition of limestone likely records times when water circulation was less restricted and reducing conditions less extreme.

The smaller cycles between the limestone beds occur on the order of 20 to 40 cm and are related to dilution of organic carbon (and most other constituents as well) by SiO_2. These cycles likely are controlled by processes related to the silica budget (Broecker and Peng, 1982).

References

Bates, R.L. and Jackson, J.A., eds., 1980, *Glossary of Geology, Second Edition*. Falls Church, American Geological Institute, p. 360.

Bray, E.E., and Evans, E.D., 1961, Distribution of n-paraffins as a clue to recognition of source beds: Geochimica et Cosmochimica Acta, 22, p. 2-15.

Brocker, W.S., and Peng, T.,1982, *Tracers in the Sea*. Palisades, Columbia University, 690 p.

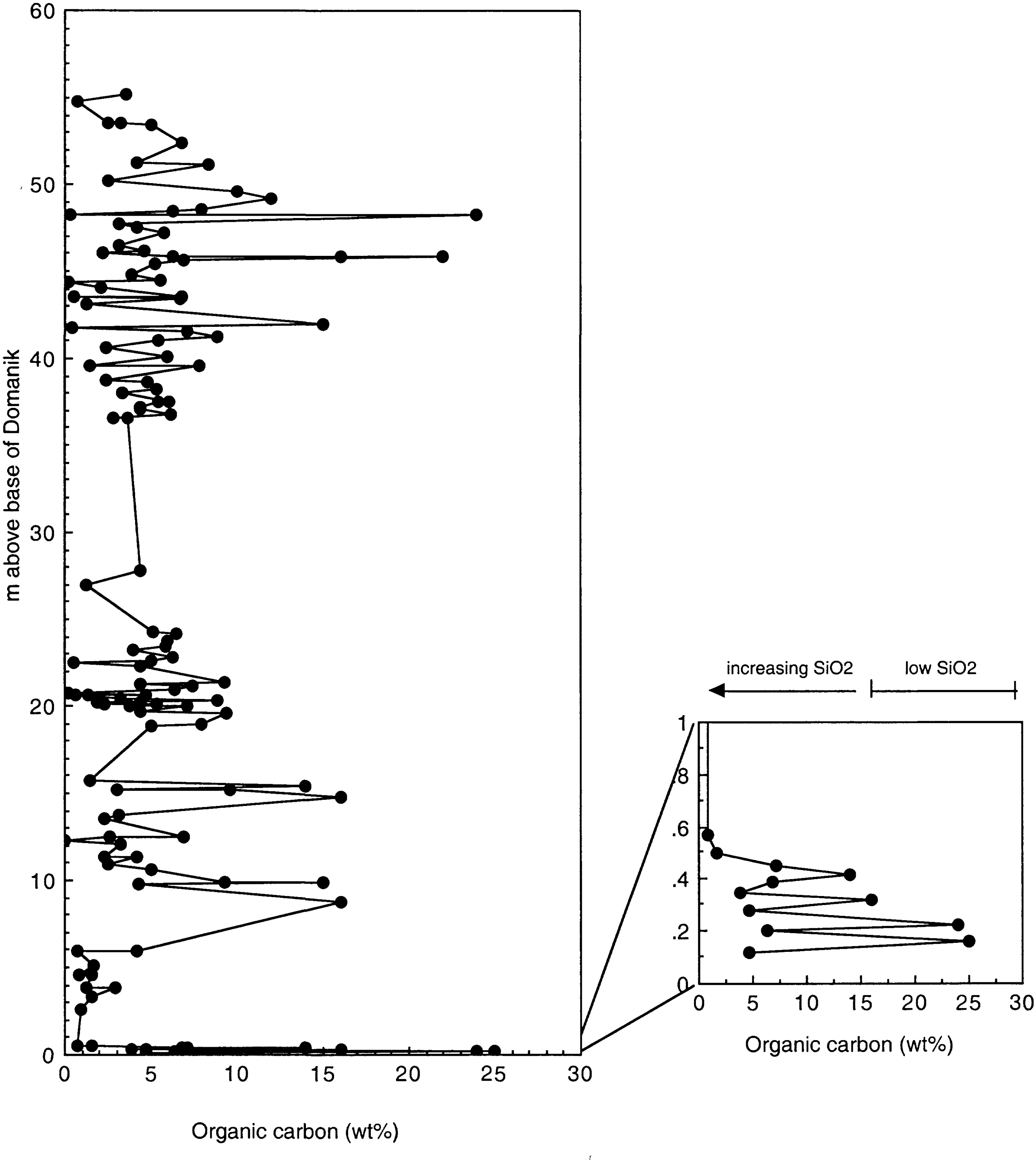


Figure 15. Depth profile of organic carbon (wt. %) for entire Domanik section sampled and 0.6 meter cycle within the Lower Domanik Formation.

Chester, R., and Aston, S.R., 1976, Geochemistry of deep-sea sediments, *in*, Riley, J.P., and Chester, R. (eds.), *Chemical Oceanography, Volume 6*. New York, Academic Press, p. 281-390.

Dean, W.E., Arthur, M.A., Stow, D.A.V., 1984, Origin and geochemistry of Cretaceous deep-sea black shales and multicolored claystones, with emphasis on Deep Sea Drilling Project Site 530, in, Hay, W.W., Sibuet J.C., et al., *Initial Reports of the Deep Sea Drilling Project, Volume LXXV*. Washington, U.S. Government Printing Office, p. 819-843.

Espitalie, J., Madec, M., Tissot, B., Mennig, J.J., and Leplat, P., 1977, Source rock characterization method for petroleum exploration: Proceedings of the 9^{th}. Annual Offshore Technology Conference, 3, p. 439-448.

Fry, B., Jannasch, H.W., Moyneaux, S.J., Wirsen, C.O., Muramoto, J.A., and King, S., 1991, Stable isotope studies of the carbon, nitrogen, and sulfur cycles in the Black Sea and the Cariaco Trench: Deep-Sea Research, 38, p. 1003-1019.

Hatch, J.R., and Leventhal, J.S., 1992, Relationship between inferred redox potential of the depositional environment and geochemistry of the Upper Pennsylvanian (Missourian) Stark Shale Member of the Dennis Limestone, Wabaunsee County, Kansas, U.S.A.: Chemical Geology,, 99, p. 65-82.

Hirst, D.M., 1974, Geochemistry of sediment from eleven Black Sea cores, in Degens, E.T., and Ross, D.A., (eds.), The Black Sea--Geology, Chemistry and Biology: American Association of Petroleum Geologist Memoir 20, p. 430-455.

Hunt, J.M., 1979, *Petroleum Geology and Geochemistry*. San Francisco, Freeman and Company, 617 p.

Hunt, J.M., 1996, *Petroleum Geology and Geochemistry, Second Edition*. San Francisco, Freeman and Company, 743 p.

Hunt, J.M., and McNichol, A.P., 1984, The Cretaceous Austin Chalk of South Texas—-a petroleum source rock, *in*, Palacas, J.G., ed., *Petroleum Geochemistry and Source Rock Potential of Carbonate Rocks: American Association of Petroleum Geologist's Studies in Geology #18*: Tulsa, American Association of Petroleum Geologist's, p. 117-125.

Krauskopf, K.B., 1979, *Introduction to Geochemistry*. New York, McGraw-Hill Book Company, 617 p.

Langford, F.F., and Blanc-Valleron, M.M., 1990, Interpreting Rock-Eval pyrolysis data using graphs of pyrolyzable hydrocarbons vs. total organic carbon: American Association of Petroleum Geologist's Bulletin, 74, p. 799-804.

Lewan, M.D., 1984, Factors controlling the proportionality of vanadium to nickel in crude oils: Geochimica et Cosmochimica Acta, 48, p. 2231-2238.

Lewan, M.D. and Maynard, J.B., 1982, Factors controlling enrichment of vanadium and nickel in the bitumen of organic sedimentary rocks: Geochimica et Cosmochimica Acta, 46, p. 2547-2560.

Manheim, F.T., 1961. A geochemical profile in the Baltic Sea: Geochimica et Cosmochimica Act, 25, p. 52-71.

Marzi, R., Torkelson, B.E., and Olson, R.K., 1993, A revised carbon preference index: Organic Geochemistry, 20, p. 1303-1306.

Orr, W.L., 1986, Kerogen/asphaltene/sulfur relationships in sulfur-rich Monterey oils: Organic Geochemistry, 10, p. 499-516.

Peters, K.E., 1986, Guidelines for evaluating petroleum source rock using programmed pyrolysis: American Association of Petroleum Geologist's Bulletin, 70, p. 318-329.

Peters, K.E., and Moldowan, J.M., 1993, *The Biomarker Guide—Interpreting Molecular Fossils in Petroleum and Ancient Sediments*. New York, Prentice Hall, 363 p.

Philippi, G.T., 1965, On the depth, time and mechanism of petroleum generation: Geochimica et Cosmochimica Acta, 29, p. 1021-1049.

Philp, R.P., 1985, *Fossil Fuel Biomarkers—Applications and Spectra*. Amsterdam, Elsevier, 294 p.

Powell, T.G., 1984, Some aspects of the hydrocarbon geochemistry of a Middle Devonian barrier-reef complex, Western Canada, *in*, Palacas, J.G., ed., *Petroleum Geochemistry and Source Rock Potential of Carbonate Rocks: American Association of Petroleum Geologist's Studies in Geology #18*. Tulsa, American Association of Petroleum Geologist's, p. 45-61.

Sælen, G., Raiswell, R., Talbot, M.R., Skei, N.M., Bottrell S.H., 1993, Heavy sedimentary sulfur isotopes as indicators of super-anoxic bottom-water conditions: Geology, 21, p. 1091-1094.

Scalan, R.S., and Smith, J.E., 1970, An improved measure of the odd-even predominance in the normal alkanes of sediment extracts and petroleum: Geochimica et Cosmochimica Acta, 34, p. 611-619.

Tissot, B.P., Durand, B., Espitalie, J., and Combax, A., 1974, Influence of nature and diageneisis of organic matter in formation of petroleum: American Association of Petroleum Geologist's Bulletin, 58, p. 499-506.

Tissot, B.P., and Welte, D.H., 1984, *Petroleum Formation and Occurrence*. Berlin, Springer-Verlag, 699 p.

Tuttle, M.L., 1988, Geochemical evolution and depositional History of Sediment in Modern and Ancient Saline Lakes: evidence from sulfur geochemistry. Unpublished Ph.D. dissertation, Colorado School of Mines, 312 p.

Tuttle, M.L., Goldhaber, M.B., Williamson, D.L., 1986, An analytical scheme for determining forms of sulphur in oil shales and associated rocks: Talanta, 33, p. 953-961.

Ulmishek, G., 1982, Petroleum geology and resource assessment of the Timan-Pechora Basin, USSR, and the adjacent Barents-Northern Kara Shelf: Argonne National Laboratory Report ANL/EES-TM-199, 197 p.
Ulmishek, G.F., 1988, Upper Devonian-Tournaisian facies and oil resources of the Russian craton's eastern margin, *in*, McMillan, N.N., Embry, A.F., Glass, D.J., eds., *Devonian of the World, Volume I: Regional Syntheses*. Calgary, Canadian Society of Petroleum Geologists, p. 527-549.
Zaback, D.A., and Pratt, L.M., 1992, Isotopic composition and speciation of sulfur in the Miocene Monterey Formation: Reevaluaation of sulfur reactions during early diagenesis in marine environments: Geochimica Cosmochimica Acta, 56, pp. 763-774.

Table A1. Data on outcrop samples collected 1994, including Rock Eval data, inorganic chemistry, and sulfur speciation and their isotopic composition. Ar, analysis done on aqua regia extract; tot, analysis done on whole rock; %, weight basis; calc, calculated. Sulfur isotopes reported relative to Cañon Diablo Troilite standard.

Sample id	Field No.	m above base	Locality	Age	Lithology	Color	T_{MAX} °C	S1 mg/gm	S2 mg/gm
94087-001	TP-01	24.20	Old Motor Road Q.	M. Domanik	massive shale	brown	423	1.8	32
94087-002	TP-02	23.80	Old Motor Road Q.	M. Domanik	massive shale	brown	423	3.3	35
94087-003	TP-04	23.20	Old Motor Road Q.	M. Domanik	massive shale	brown	428	1.5	22
94087-004	TP-05	22.80	Old Motor Road Q.	M. Domanik	massive shale	brown	422	2.7	39
94087-005	TP-06	21.40	Old Motor Road Q.	M. Domanik	fissile shale	gray	428	2.6	48
94087-006	TP-07	21.10	Old Motor Road Q.	M. Domanik	fissile shale	brown	426	2.3	39
94087-007	TP-08	20.60	Old Motor Road Q.	M. Domanik	massive shale	brown	428	0.57	9.1
94087-008	TP-9A gray	20.20	Old Motor Road Q.	M. Domanik	massive shale	gray	425	1.3	15
94087-009	TP-9A brown	20.10	Old Motor Road Q.	M. Domanik	massive shale	brown	424	2.5	34
94087-010	TP-09	20.15	Old Motor Road Q.	M. Domanik	massive shale	brown	428	0.89	12
94087-011	TP-10	5.94	Outcrop 7	L. Domanik	fissile shale	brown	434	0	14
94087-012	TP-11	5.11	Outcrop 7	L. Domanik	massive shale	brown	428	0.76	9.5
94087-013	TP-12	4.61	Outcrop 7	L. Domanik	massive shale	brown	424	0.53	6
94087-014	TP-13	3.90	Outcrop 7	L. Domanik	massive shale	gray	429	0.53	8
94087-015	TP-14	3.30	Outcrop 7	L. Domanik	limestone	brown	428	0.78	8
94087-016	TP-15	2.60	Outcrop 7	L. Domanik	massive shale	brown	431	0.37	4.5
94087-017	TP-17 brown	11.33	Outcrop 7	L. Domanik	massive shale	brown	427	1.2	25
94087-018	TP-17 gray	11.38	Outcrop 7	L. Domanik	massive shale	gray	429	1.1	14
94087-019	TP-18	12.54	Outcrop 7	L. Domanik	massive shale	brown	428	0.53	14
94087-020	TP-19	9.85	Outcrop 7	L. Domanik	massive shale	brown	423	4.5	56
94087-021	TP-20	40.60	Outcrop 21	M. - U. Domanik	massive shale	gray	426	0.77	14
94087-022	TP-21	43.10	Outcrop 21	M. - U. Domanik	massive shale	brown	431	0.46	8.5
94087-023	TP-22	44.10	Outcrop 21	M. - U. Domanik	massive shale	brown	425	0.83	9.0
94087-024	TP-23	45.80	Outcrop 21	M. - U. Domanik	fissile shale	brown	416	11	141
94087-025	TP-24 brown	46.14	Black Dog Q.	M. - U. Domanik	massive shale	brown	424	2.6	31
94087-026	TP-24 gray	46.09	Black Dog Q.	M. - U. Domanik	massive shale	gray	426	1.6	16
94087-027	TP-25	47.19	Black Dog Q.	M. - U. Domanik	fissile shale	brown	421	3.5	40
94087-028	TP-26	48.19	Black Dog Q.	M. - U. Domanik	fissile shale	brown	418	13	159
94087-029	TP-27	52.39	Black Dog Q.	M. - U. Domanik	fissile shale	brown	422	1.5	40
94087-030	TP-28 black	53.54	Black Dog Q.	M. - U. Domanik	massive shale	brown	427	1.2	16
94087-031	TP-28 gray	53.59	Black Dog Q.	M. - U. Domanik	massive shale	gray	431	0.85	9.6

Table A1. Continued.

Sample id	TOC %	HI	OI	Tot S %	Na % (AR)	Tot Na %	Mg % (AR)	Tot Mg %	Al % (AR)	Tot Al%	P% (AR)	Tot P %
94087-001	6.5	484	96	0.32	0.02	0.06	0.09	0.14	0.07	0.79	0.06	0.07
94087-002	5.9	595	102	0.41	0.03	nd	0.11	nd	0.11	nd	0.06	nd
94087-003	4.0	553	102	0.25	0.03	0.06	0.16	0.26	0.07	0.86	0.07	0.07
94087-004	6.2	631	73	0.36	0.02	0.07	0.08	0.18	0.08	1.0	0.06	0.07
94087-005	9.3	524	64	0.70	0.02	0.06	0.07	0.26	0.14	1.5	0.09	0.09
94087-006	7.4	526	68	0.55	0.02	0.05	0.15	0.31	0.13	1.5	0.09	0.09
94087-007	1.4	661	114	0.21	0.02	0.07	0.01	0.02	0.02	0.28	0.02	0.03
94087-008	1.9	634	132	0.40	0.02	0.07	0.39	0.31	0.04	0.81	0.03	0.07
94087-009	5.3	650	89	0.30	nd	0.05	nd	0.40	nd	0.46	nd	0.03
94087-010	2.3	664	107	0.26	0.02	0.06	0.02	0.04	0.03	0.29	0.03	0.03
94087-011	4.2	340	108	0.21	0.03	0.06	0.19	0.39	0.18	1.6	0.08	0.08
94087-012	1.7	552	141	0.26	0.02	0.07	0.04	0.07	0.06	0.49	0.03	0.04
94087-013	0.79	797	96	0.22	0.03	0.08	0.02	0.03	0.02	0.27	0.03	0.03
94087-014	1.3	577	139	0.23	0.02	0.07	0.01	0.03	0.02	0.32	0.02	0.02
94087-015	1.6	499	158	0.32	0.02	0.04	0.25	0.30	0.06	0.40	0.05	0.05
94087-016	0.93	486	148	0.16	0.03	0.07	<0.01	0.01	0.02	0.24	0.02	0.02
94087-017	4.2	581	116	0.27	0.02	0.07	0.10	0.16	0.07	0.74	0.05	0.05
94087-018	2.3	598	103	0.19	0.02	0.07	0.06	0.08	0.04	0.45	0.03	0.04
94087-019	2.6	548	157	0.20	0.02	0.09	0.14	0.21	0.09	0.98	0.06	0.06
94087-020	9.3	596	43	1.1	0.02	0.05	0.29	0.22	0.11	1.2	0.11	0.11
94087-021	2.4	565	100	0.28	0.02	0.06	0.01	0.05	0.05	0.49	0.04	0.05
94087-022	1.3	635	121	0.36	0.02	0.06	0.01	0.04	0.03	0.35	0.02	0.02
94087-023	2.1	439	78	0.33	0.02	0.06	0.01	0.04	0.04	0.40	0.03	0.03
94087-024	22	639	38	0.90	0.03	0.05	0.67	0.81	0.11	1.1	0.10	0.10
94087-025	4.6	678	67	0.26	0.02	0.06	0.11	0.28	0.10	0.98	0.05	0.06
94087-026	2.2	727	95	0.39	nd	0.06	nd	0.35	nd	0.63	nd	0.04
94087-027	5.7	698	50	0.41	0.03	0.07	0.10	0.18	0.13	1.0	0.06	0.06
94087-028	24	656	17	1.4	nd	0.04	nd	0.93	nd	0.83	nd	0.10
94087-029	6.8	592	25	1.6	0.02	0.08	0.13	0.61	0.28	4.7	0.05	0.06
94087-030	3.2	493	90	0.21	0.02	0.06	0.02	0.04	0.04	0.37	0.02	0.02
94087-031	2.5	384	109	0.20	0.02	0.06	0.03	0.05	0.05	0.39	0.02	0.03

Table A1. Continued.

Sample id	K% (AR)	Tot K %	Ca % (AR)	Tot Ca %	Sc ppm (AR)	Tot Sc ppm	Tot Ti %	V ppm (AR)	Tot V ppm	Cr ppm (AR)
94087-001	0.06	0.24	8.5	9.9	1.0	1.6	0.03	67	106	8
94087-002	0.08	nd	11	nd	1.3	nd	nd	116	nd	12
94087-003	0.05	0.38	16	17	1.6	2.3	0.05	200	357	6
94087-004	0.06	0.39	7.8	8.3	1.7	2.3	0.06	261	500	8
94087-005	0.11	0.58	4.1	4.7	1.5	3.2	0.07	564	1160	21
94087-006	0.09	0.52	9.9	10	2.6	3.7	0.07	374	652	14
94087-007	0.01	0.09	0.67	0.83	<0.5	0.6	0.01	160	205	20
94087-008	0.03	0.28	12	7.6	1.0	1.9	0.04	158	386	8
94087-009	nd	0.13	nd	13	nd	1.2	0.02	nd	199	nd
94087-010	0.02	0.10	1.5	1.8	<0.5	0.7	0.01	242	328	24
94087-011	0.12	0.56	16	19	2.2	3.8	0.09	91	258	8
94087-012	0.04	0.17	2.6	3.0	0.5	1.1	0.02	191	267	27
94087-013	0.01	0.09	1.5	1.6	<0.5	0.5	0.01	74	102	21
94087-014	0.01	0.08	1.1	1.4	<0.5	0.5	0.01	94	116	24
94087-015	0.04	0.19	23	26	1.0	1.4	0.02	118	153	4
94087-016	0.01	0.07	0.15	0.22	<0.5	<0.5	0.01	106	125	26
94087-017	0.05	0.22	10	12	2.0	2.3	0.03	102	235	6
94087-018	0.03	0.14	4.9	5.7	0.6	1.1	0.03	77	152	13
94087-019	0.05	0.33	12	14	1.3	2.1	0.07	134	329	7
94087-020	0.07	0.43	9.1	9.3	1.9	2.5	0.06	519	789	11
94087-021	0.04	0.18	1.0	1.4	<0.5	1.1	0.02	176	317	31
94087-022	0.02	0.11	1.3	1.6	<0.5	0.8	0.01	136	223	22
94087-023	0.03	0.14	0.78	0.93	<0.5	0.7	0.02	242	364	27
94087-024	0.09	0.42	15	17	1.4	2.5	0.05	67	89	7
94087-025	0.07	0.34	8.1	9.5	1.4	2.0	0.04	238	417	11
94087-026	nd	0.22	nd	16	nd	1.5	0.03	nd	284	nd
94087-027	0.09	0.34	8.8	9.4	1.7	2.3	0.05	335	588	11
94087-028	nd	0.33	nd	17	nd	2.4	0.04	nd	79	nd
94087-029	0.17	1.2	7.3	7.6	3.1	7.6	0.27	105	322	10
94087-030	0.03	0.12	1.3	1.5	<0.5	0.7	0.02	210	320	18
94087-031	0.03	0.13	1.9	2.1	0.6	0.9	0.02	183	276	17

Table A1. Continued.

Sample id	Tot Cr ppm	Mn ppm (AR)	Tot Mn ppm	Fe % (AR)	Tot Fe %	Co ppm (AR)	Tot Co ppm	Ni ppm (AR)	Tot Ni ppm
94087-001	16	65	64	0.28	0.35	2	2	48	49
94087-002	nd	76	nd	0.88	nd	4	nd	62	nd
94087-003	13	61	59	0.20	0.27	2	<1	61	58
94087-004	32	34	34	0.23	0.31	3	1	70	66
94087-005	30	94	94	0.58	0.76	5	5	141	141
94087-006	49	24	28	0.51	0.62	2	1	113	106
94087-007	30	11	12	0.21	0.24	<1	<1	27	28
94087-008	25	30	38	0.15	0.34	1	1	32	67
94087-009	14	nd	29	nd	0.17	nd	<1	nd	29
94087-010	33	18	18	0.27	0.30	<1	<1	42	44
94087-011	29	263	259	0.51	0.76	2	2	109	111
94087-012	10	29	27	0.38	0.42	1	<1	42	44
94087-013	7	19	19	0.26	0.26	2	<1	20	22
94087-014	29	27	28	0.31	0.35	1	<1	28	31
94087-015	12	118	112	0.20	0.24	3	1	43	39
94087-016	13	17	18	0.37	0.41	2	<1	31	34
94087-017	17	75	74	0.35	0.43	3	1	61	61
94087-018	9	31	35	0.20	0.30	1	<1	47	49
94087-019	16	94	87	0.73	0.78	3	2	69	64
94087-020	38	43	44	0.29	0.33	3	4	87	88
94087-021	35	19	18	0.32	0.28	2	<1	31	35
94087-022	31	17	15	0.43	0.46	1	<1	23	25
94087-023	38	12	13	0.29	0.33	<1	<1	35	39
94087-024	15	116	116	0.60	0.76	6	5	40	39
94087-025	26	43	41	0.26	0.29	2	1	43	48
94087-026	17	nd	62	nd	0.17	nd	2	nd	30
94087-027	27	45	44	0.19	0.27	2	<1	68	63
94087-028	12	nd	105	nd	1.3	nd	7	nd	40
94087-029	71	66	72	1.4	1.9	8	7	160	153
94087-030	20	17	18	0.27	0.31	2	<1	71	78
94087-031	7	36	28	0.46	0.39	2	1	67	68

Table A1. Continued.

Sample id	Cu ppm (AR)	Tot Cu ppm	Zn ppm (AR)	Tot Zn ppm	As ppm (AR)	Tot As ppm	Sr ppm (AR)	Tot Sr ppm	Y ppm (AR)
94087-001	25	22	15	15	3	8	327	517	13
94087-002	38	nd	185	nd	18	nd	407	nd	18
94087-003	23	18	61	57	5	<3	531	518	28
94087-004	34	28	69	66	7	9	238	245	22
94087-005	85	78	240	255	11	16	109	141	23
94087-006	75	64	240	225	11	17	233	235	29
94087-007	16	16	31	40	5	4	17	33	5.8
94087-008	23	48	46	114	7	4	178	198	11
94087-009	nd	19	nd	43	nd	5	nd	182	nd
94087-010	24	23	45	50	<3	6	39	60	7.9
94087-011	25	21	30	32	<3	<3	569	589	24
94087-012	24	23	82	89	<3	<3	49	59	9.0
94087-013	15	14	50	60	<3	6	26	33	5.1
94087-014	18	18	50	58	4	4	19	30	4.3
94087-015	18	12	89	80	7	3	260	243	12
94087-016	17	16	67	80	<3	<3	4.1	12	3.1
94087-017	17	14	74	75	4	8	318	349	25
94087-018	12	9.6	23	24	<3	6	158	183	14
94087-019	35	29	218	209	6	<3	429	428	24
94087-020	62	46	139	155	8	<3	242	255	27
94087-021	20	22	27	37	<3	4	28	60	9.8
94087-022	18	18	32	36	6	3	31	49	6.8
94087-023	20	20	56	64	3	<3	34	52	6.2
94087-024	63	57	30	32	7	7	529	559	19
94087-025	31	29	63	81	5	<3	198	237	17
94087-026	nd	15	nd	48	nd	8	nd	349	nd
94087-027	34	29	116	110	5	9	336	384	21
94087-028	nd	70	nd	22	nd	<3	nd	551	nd
94087-029	51	42	259	257	10	<3	274	314	20
94087-030	23	23	144	169	5	6	59	90	6.9
94087-031	21	19	110	120	6	4	77	104	9.6

Table A1. Continued.

Sample id	Tot Y ppm	Zr ppm (AR)	Tot Zr ppm	Tot Mo ppm	Ag ppm (AR)	Ba ppm (AR)	Tot Ba ppm	La ppm (AR)	Tot La ppm
94087-001	13	4.4	16	13	<0.2	12	63	7.8	8.4
94087-002	nd	5.7	nd	nd	0.4	15	nd	8.9	nd
94087-003	26	7.1	20	7	0.4	10	54	16	14
94087-004	21	6.7	27	10	0.9	10	61	11	10
94087-005	24	11	42	15	1.2	14	72	12	13
94087-006	27	9.8	36	14	1.1	11	62	17	16
94087-007	6.2	3.1	9.7	5	0.4	4	20	3	2.7
94087-008	18	5.6	21	20	0.7	5	48	6.5	9.1
94087-009	9.9	nd	9.4	11	nd	nd	22	nd	5.0
94087-010	8.0	2.9	11	12	<0.2	4	21	3.3	3.4
94087-011	25	7.2	40	11	<0.2	21	84	15	17
94087-012	9.5	4.1	13	12	0.3	6	25	5	4.8
94087-013	5.0	2.6	8.1	7	<0.2	3	14	2.4	2.3
94087-014	4.9	3.7	9.3	13	0.4	4	17	3	2.5
94087-015	12	6.4	11	8	<0.2	7	27	7.5	5.5
94087-016	3.7	2.3	8.3	7	0.5	4	19	1.6	1.6
94087-017	25	5.1	21	8	0.2	17	81	13	13
94087-018	14	3.8	13	13	0.4	12	55	7.4	6.6
94087-019	23	5.7	26	16	1.2	16	76	14	14
94087-020	27	9.1	31	22	0.9	7	52	13	13
94087-021	12	3.1	14	8	0.3	4	27	4.1	5.2
94087-022	7.1	2.7	9.6	7	<0.2	2	16	3.2	3.2
94087-023	6.8	4.0	12	14	0.5	4	24	2.7	3.3
94087-024	19	11	35	11	0.9	9	47	15	17
94087-025	17	5.6	21	12	0.6	8	50	9.6	9.5
94087-026	13	nd	13	6	nd	nd	28	nd	7.0
94087-027	20	5.9	22	27	0.5	11	50	9.5	10
94087-028	18	nd	27	11	nd	nd	41	nd	14
94087-029	24	24	179	50	0.8	13	190	14	31
94087-030	7.6	4.1	13	21	0.7	7	30	2.9	3.5
94087-031	9.8	5.3	13	18	0.7	8	27	4.7	4.6

Table A1. Continued.

Sample id	Pb ppm (AR)	Tot Pb ppm	SiO_2 % (calc)	Clay % (calc)	Calcite % (calc)	$S_{monosulfide}$ %	$S_{disulfide}$ %	S_{SO4} %	$S_{organic}$ %
94087-001	4	<2	70	3.8	11	0.007	0.007	0.007	0.30
94087-002	9	nd	66	nd	14	0.007	0.041	0.007	0.35
94087-003	5	2	55	4.1	20	0.007	0.007	0.007	0.23
94087-004	4	2	73	4.9	10	0.007	0.007	0.007	0.34
94087-005	7	7	78	7.2	5.4	0.007	0.12	0.010	0.56
94087-006	5	6	66	7.2	13	0.007	0.052	0.007	0.48
94087-007	2	2	97	1.3	0.87	0.007	0.030	0.007	0.17
94087-008	<2	6	67	3.9	16	0.007	0.030	0.050	0.31
94087-009	nd	<2	94	2.2	nd	0.007	0.030	0.040	0.22
94087-010	5	<2	93	1.4	1.9	0.007	0.035	0.007	0.21
94087-011	<2	<2	54	7.7	21	0.007	0.007	0.007	0.19
94087-012	4	<2	91	2.4	3.4	0.007	0.063	0.007	0.18
94087-013	<2	<2	95	1.3	1.9	0.011	0.040	0.007	0.16
94087-014	4	<2	96	1.5	1.4	0.007	0.030	0.007	0.19
94087-015	<2	3	39	1.9	30	0.007	0.007	0.060	0.25
94087-016	24	26	99	1.2	0.21	0.007	0.025	nd	0.13
94087-017	<2	2	70	3.6	13	0.007	0.013	0.076	0.17
94087-018	3	<2	85	2.2	6.3	0.007	0.038	0.007	0.14
94087-019	5	5	65	4.7	16	0.007	0.051	0.007	0.13
94087-020	2	5	65	5.5	12	0.030	0.34	0.050	0.64
94087-021	2	3	95	2.4	1.3	0.007	0.034	0.007	0.23
94087-022	6	6	95	1.7	1.6	0.016	0.16	0.027	0.16
94087-023	2	<2	96	1.9	1.0	0.007	0.072	0.007	0.24
94087-024	7	5	34	5.2	21	0.13	0.010	0.050	0.71
94087-025	3	<2	74	4.7	10	0.020	0.020	0.007	0.21
94087-026	nd	<2	97	3.0	nd	0.010	0.090	0.020	0.27
94087-027	6	4	71	4.9	11	0.007	0.030	0.020	0.35
94087-028	nd	5	71	4.0	nd	0.020	0.52	0.040	0.81
94087-029	7	5	73	22	9.5	0.080	1.1	0.060	0.38
94087-030	<2	<2	93	1.8	1.7	0.007	0.024	0.007	0.17
94087-031	<2	<2	92	1.9	2.4	0.007	0.023	0.007	0.16

Table A1. Continued.

Sample id	$\delta^{34}S_{disulfide}$ ‰	$\delta^{34}S_{organic}$ ‰
94087-001	Insuff	16.1
94087-002	21.0	Insuff
94087-003	nd	nd
94087-004	nd	nd
94087-005	11.9	12.4
94087-006	8.5	12.3
94087-007	9.7	11.3
94087-008	9.8	14.2
94087-009	9.9	14.0
94087-010	nd	nd
94087-011	Insuff	10.7
94087-012	nd	nd
94087-013	5.4	9.5
94087-014	11.2	10.2
94087-015	Insuff	10.8
94087-016	11.9	9.2
94087-017	19.3	9.7
94087-018	2.6	8.9
94087-019	4.0	9.1
94087-020	16.2	22.5
94087-021	nd	nd
94087-022	20.8	18.4
94087-023	20.7	18.5
94087-024	2.9	22.5
94087-025	11.1	20.2
94087-026	18.4	20.0
94087-027	nd	nd
94087-028	8.8	22.0
94087-029	nd	nd
94087-030	10.9	11.3
94087-031	11.2	11.8

Table A2. Data on outcrop samples collected 1995, including Rock Eval data, inorganic chemistry. Ar, analysis done on aqua regia extract; tot, analysis done on whole rock; %, weight basis; calc, calculated.

Sample id	Field no.	m above base	Locality	Age	Lithology	Color	T_{MAX} °C	S1 mg/gm	S2 mg/gm
96018-001	UK1	0.12	Outcrop 7	L. Domanik	massive shale	brown	415	2.3	26
96018-002	UK2	0.16	Outcrop 7	L. Domanik	fissile shale	black	414	20	132
96018-003	UK3	0.20	Outcrop 7	L. Domanik	massive shale	brown	416	3.3	35
96018-004	UK4	0.22	Outcrop 7	L. Domanik	fissile shale	gray	414	19	121
96018-005	UK5	0.28	Outcrop 7	L. Domanik	massive shale	brown	418	3.7	26
96018-006	UK6	0.32	Outcrop 7	L. Domanik	fissile shale	black	416	11	75
96018-007	UK7	0.35	Outcrop 7	L. Domanik	massive shale	brown	418	3.2	20
96018-008	UK8	0.39	Outcrop 7	L. Domanik	massive shale	brown	419	5.4	38
96018-009	UK9	0.42	Outcrop 7	L. Domanik	fissile shale	gray	418	10	69
96018-010	UK10	0.45	Outcrop 7	L. Domanik	massive shale	brown	416	5.3	38
96018-011	UK11	0.57	Outcrop 7	L. Domanik	limestone	brown	426	0.32	3.2
96018-012	UK12	3.90	Outcrop 7	L. Domanik	limestone	brown	422	2.3	14
96018-013	UK13	4.61	Outcrop 7	L. Domanik	massive shale	black	423	0.81	6.9
96018-014	UK14	5.94	Outcrop 7	L. Domanik	limestone	brown	421	0.28	3.0
96018-015	UK15	8.80	Outcrop 7	L. Domanik	fissile shale	black	416	9.5	88
96018-016	UK16	9.80	Outcrop 7	L. Domanik	massive shale	brown	422	1.7	22
96018-017	UK17	9.85	Outcrop 7	L. Domanik	fissile shale	black	418	8.8	85
96018-018	UK18	10.58	Outcrop 7	L. Domanik	massive shale	brown	419	2.5	23
96018-019	UK19	10.98	Outcrop 7	L. Domanik	massive shale	brown	420	1.8	14
96018-020	UK20	12.05	Outcrop 7	L. Domanik	massive shale	brown	423	1.2	15
96018-021	UK21	12.30	Outcrop 7	L. Domanik	limestone	brown	423	0.01	0.11
96018-022	UK22	12.54	Outcrop 7	L. Domanik	massive shale	brown	422	0.91	26
96018-023	UK23	13.50	Outcrop 7	L. Domanik	limestone	brown	419	1.4	13
96018-024	UK24	13.76	Outcrop 7	L. Domanik	massive shale	brown	420	1.3	18
96018-026	UK26	14.76	Outcrop 7	L. Domanik	fissile shale	brown	416	10	85
96018-027	UK27	15.22	Outcrop 7	L. Domanik	massive shale	brown	414	6.5	52
96018-028	UK28	15.25	Outcrop 7	L. Domanik	massive shale	black	416	1.7	16
96018-029	UK29	15.45	Outcrop 7	L. Domanik	massive shale	brown	417	7.8	82
96018-030	UK30	15.70	Outcrop 7	L. Domanik	limestone	brown	420	0.33	5.8
96018-031	UK31A	20.67	Outcrop 7	L. Domanik	massive shale	brown	423	1.7	22
96018-032	UK31B	20.00	Outcrop 7	L. Domanik	limestone	brown	422	1.3	20

Table A2. Continued.

Sample id	S3 mg/gm	PI	S2/S3	PC	TOC %	HI	OI	Total S %	Na % (AR)	Tot Na %	Mg % (AR)	Tot Mg %
96018-001	1.4	0.08	18	2.4	4.7	556	30	0.46	0.03	0.08	0.01	0.04
96018-002	6.7	0.13	20	13	25	520	26	2.26	0.04	0.08	0.12	0.32
96018-003	1.7	0.09	21	3.2	6.4	550	26	0.50	0.03	0.08	0.02	0.06
96018-004	4.1	0.14	30	12	24	510	17	2.2	0.04	0.06	0.12	0.29
96018-005	0.72	0.12	36	2.5	4.7	561	15	1.1	0.03	0.08	0.02	0.06
96018-006	3.7	0.13	20	7.2	16	477	23	1.3	0.03	0.06	0.12	0.26
96018-007	0.58	0.14	35	1.9	3.9	511	14	1.2	0.03	0.07	0.02	0.05
96018-008	1.0	0.13	38	3.6	6.8	548	14	0.72	0.03	0.08	0.06	0.10
96018-009	2.1	0.13	34	6.6	14	485	14	1.1	0.03	0.07	0.12	0.27
96018-010	1.3	0.12	29	3.6	7.1	540	18	0.73	0.03	0.08	0.06	0.12
96018-011	0.44	0.09	7.3	0.29	0.77	418	57	0.13	0.02	0.02	0.32	0.33
96018-012	0.63	0.14	23	1.4	2.9	506	22	0.37	0.02	0.04	0.19	0.24
96018-013	0.67	0.10	10	0.64	1.6	442	42	0.22	0.03	0.07	0.05	0.07
96018-014	0.26	0.08	12	0.27	0.69	439	37	0.14	0.02	0.03	0.25	0.30
96018-015	2.8	0.10	32	8.1	16	555	17	1.7	0.02	0.06	0.25	0.40
96018-016	1.9	0.07	12	1.9	4.3	507	43	0.29	0.03	0.06	0.14	0.22
96018-017	3.3	0.09	26	7.9	15	555	21	1.6	0.02	0.06	0.15	0.27
96018-018	1.8	0.10	13	2.1	5.0	453	36	0.39	0.03	0.06	0.17	0.31
96018-019	0.63	0.12	22	1.3	2.5	544	25	0.41	0.02	0.06	0.09	0.14
96018-020	1.4	0.07	10	1.3	3.2	466	44	0.23	0.02	0.07	0.06	0.18
96018-021	0.09	0.08	1.2	0.01	0.02	550	450	0.035	0.02	0.02	0.39	0.40
96018-022	2.9	0.03	8.9	2.3	6.9	381	42	0.41	0.03	0.07	0.17	0.50
96018-023	0.72	0.09	18	1.2	2.3	564	30	0.13	0.02	0.04	0.18	0.23
96018-024	1.1	0.07	16	1.6	3.1	565	36	0.29	0.02	0.05	0.09	0.15
96018-026	1.9	0.11	45	7.9	16	537	12	1.8	0.03	0.05	0.19	0.30
96018-027	2.0	0.11	27	4.9	9.6	545	20	0.91	0.03	0.05	0.19	0.26
96018-028	0.55	0.10	29	1.5	3.0	538	18	1.0	0.02	0.07	0.12	0.15
96018-029	2.2	0.09	37	7.5	14	594	15	1.5	0.03	0.05	0.15	0.25
96018-030	0.66	0.05	8.8	0.5	1.5	393	44	0.60	0.02	0.03	0.24	0.28
96018-031	2.0	0.07	11	2.0	4.7	466	41	0.43	0.03	0.07	0.15	0.24
96018-032	1.5	0.06	13	1.8	3.7	542	41	0.42	0.03	0.06	0.08	0.14

Table A2. Continued.

Sample id	Al % (AR)	Tot Al%	P% (AR)	Tot P %	K% (AR)	Tot K %	Ca % (AR)	Tot Ca %	Sc ppm (AR)	Tot Sc ppm	Tot Ti %
96018-001	0.03	0.47	0.03	0.04	0.02	0.13	0.76	0.89	<0.5	0.8	0.02
96018-002	0.18	2.2	0.19	0.20	0.08	0.68	6.1	7.3	2.9	5.4	0.11
96018-003	0.04	0.53	0.04	0.04	0.02	0.17	1.6	1.8	0.7	1.0	0.02
96018-004	0.16	2.0	0.12	0.13	0.08	0.62	7.1	8.4	2.5	5.0	0.10
96018-005	0.03	0.5	0.02	0.03	0.02	0.16	1.3	1.7	0.6	1.0	0.02
96018-006	0.13	1.7	0.11	0.11	0.06	0.53	9.0	11	2.4	4.3	0.09
96018-007	0.03	0.42	0.02	0.03	0.02	0.13	1.5	1.9	<0.5	0.9	0.02
96018-008	0.06	0.66	0.05	0.04	0.03	0.27	4.3	4.6	1.1	1.2	0.04
96018-009	0.13	1.9	0.09	0.10	0.06	0.56	9.2	12	2.1	4.2	0.09
96018-010	0.06	0.74	0.04	0.05	0.03	0.26	4.4	5.3	1.1	1.9	0.04
96018-011	0.01	0.17	0.01	0.01	0.01	0.04	31	34	<0.5	0.6	<0.01
96018-012	0.04	0.45	0.04	0.04	0.03	0.17	24	28	1.1	1.5	0.02
96018-013	0.03	0.33	0.04	0.05	0.02	0.10	4.9	6.2	0.6	0.8	0.01
96018-014	0.03	0.39	0.03	0.03	0.03	0.16	28	33	0.6	1.3	0.02
96018-015	0.07	1.1	0.08	0.09	0.06	0.45	7.8	9.3	1.0	2.2	0.05
96018-016	0.05	0.79	0.04	0.05	0.05	0.33	14	16	1.0	1.6	0.04
96018-017	0.07	1.1	0.07	0.08	0.07	0.47	7.4	9.0	1.0	2.3	0.05
96018-018	0.11	1.2	0.09	0.09	0.08	0.52	15	17	1.8	2.9	0.07
96018-019	0.04	0.50	0.07	0.07	0.04	0.20	7.6	8.6	0.8	1.2	0.02
96018-020	0.07	1.1	0.04	0.05	0.06	0.41	4.5	5.7	2.9	4.0	0.07
96018-021	<0.01	0.04	0.04	0.04	<0.01	<0.01	32	36	<0.5	0.5	<0.01
96018-022	0.25	2.9	0.07	0.07	0.17	1.23	12	14	2.0	5.1	0.15
96018-023	0.04	0.50	0.02	0.03	0.04	0.20	21	25	0.7	1.2	0.03
96018-024	0.04	0.61	0.03	0.04	0.04	0.24	10	13	0.7	1.3	0.03
96018-026	0.06	0.81	0.10	0.11	0.05	0.33	16	19	1.0	1.9	0.04
96018-027	0.04	0.56	0.08	0.08	0.04	0.23	19	24	0.8	1.5	0.03
96018-028	0.01	0.25	0.03	0.03	0.02	0.08	4.4	5.0	<0.5	0.5	0.01
96018-029	0.06	0.77	0.10	0.11	0.05	0.31	15	19	1.0	1.9	0.04
96018-030	<0.01	0.12	0.02	0.02	0.01	0.03	28	35	<0.5	0.5	<0.01
96018-031	0.07	0.80	0.08	0.09	0.04	0.29	10	13	1.3	1.8	0.04
96018-032	0.03	0.55	0.04	0.04	0.03	0.18	6.8	8.8	0.9	1.4	0.02

Table A2. Continued.

Sample id	V ppm (AR)	Tot V ppm	Cr ppm (AR)	Tot Cr ppm	Mn ppm (AR)	Tot Mn ppm	Fe % (AR)	Tot Fe %	Co ppm (AR)
96018-001	84	115	2	7	14	21	0.36	0.46	2
96018-002	349	593	11	40	92	99	1.29	1.66	6
96018-003	92	101	2	7	36	34	0.33	0.39	3
96018-004	261	402	9	33	103	111	1.26	1.51	10
96018-005	87	112	2	8	35	38	0.80	1.27	2
96018-006	273	437	8	31	121	130	0.81	1.01	5
96018-007	71	118	2	5	27	28	0.93	0.95	1
96018-008	127	180	3	12	57	51	0.42	0.52	3
96018-009	227	438	7	31	100	112	0.63	0.86	5
96018-010	131	206	4	15	58	59	0.44	0.53	3
96018-011	35	48	1	1	182	188	0.14	0.14	<1
96018-012	116	142	9	11	64	62	0.14	0.18	1
96018-013	86	111	4	3	21	23	0.12	0.15	1
96018-014	46	73	2	6	58	58	0.17	0.2	1
96018-015	63	89	5	14	169	174	0.70	0.85	6
96018-016	71	106	2	10	100	105	0.20	0.28	1
96018-017	62	88	4	13	145	152	0.61	0.78	6
96018-018	348	688	8	35	54	55	0.29	0.41	2
96018-019	144	229	4	13	27	28	0.18	0.26	1
96018-020	163	383	4	22	24	27	0.27	0.39	2
96018-021	17	16	1	<1	79	79	0.05	0.05	<1
96018-022	284	726	9	43	66	75	0.61	0.95	2
96018-023	113	190	3	8	77	79	0.10	0.15	<1
96018-024	53	83	1	7	151	183	0.19	0.25	4
96018-026	50	66	4	10	215	214	0.65	0.77	7
96018-027	35	47	2	7	241	247	0.38	0.48	5
96018-028	12	16	1	3	58	59	0.56	0.63	2
96018-029	39	57	3	9	220	233	0.47	0.63	6
96018-030	8	9	<1	<1	339	367	0.49	0.44	1
96018-031	283	505	7	25	40	45	0.23	0.31	1
96018-032	162	236	4	11	27	32	0.23	0.3	<1

Table A2. Continued.

Sample id	Tot Co ppm	Ni ppm (AR)	Tot Ni ppm	Cu ppm (AR)	Tot Cu ppm	Zn ppm (AR)	Tot Zn ppm	As ppm (AR)
96018-001	2	52	58	17	16	359	438	3
96018-002	6	200	202	121	124	615	636	12
96018-003	2	64	61	25	22	362	313	5
96018-004	9	167	168	109	108	215	212	11
96018-005	2	37	40	25	29	33	36	8
96018-006	6	107	109	79	78	105	86	8
96018-007	2	30	40	22	23	52	64	6
96018-008	2	47	46	38	31	29	24	7
96018-009	5	85	93	69	72	42	46	7
96018-010	2	48	53	37	36	52	54	5
96018-011	<1	13	12	7.1	<0.5	61	53	-3
96018-012	<1	32	31	25	19	68	64	4
96018-013	<1	24	27	21	20	54	57	-3
96018-014	<1	12	13	11	3.3	41	41	4
96018-015	6	41	43	64	63	11	15	7
96018-016	2	40	40	22	18	1.7	2.0	5
96018-017	6	42	44	58	57	6.0	7.0	5
96018-018	2	108	105	52	47	219	204	8
96018-019	<1	29	30	17	16	54	59	<3
96018-020	2	54	59	28	27	81	85	<3
96018-021	<1	12	11	3.8	<0.5	14	9.9	<3
96018-022	2	111	110	68	64	296	284	9
96018-023	<1	23	25	12	7.3	15	13	<3
96018-024	4	36	40	17	15	5.4	5.7	4
96018-026	6	28	29	46	41	7.9	7.8	4
96018-027	4	18	19	32	29	5.3	4.1	7
96018-028	3	6	11	12	12	1.4	1.1	3
96018-029	6	27	31	49	49	8.3	8.1	5
96018-030	<1	3	4	6.4	<0.5	1.6	<0.5	4
96018-031	1	61	65	30	29	121	119	6
96018-032	1	40	45	24	23	75	82	7

Table A2. Continued.

Sample id	Tot As ppm	Sr ppm (AR)	Tot Sr ppm	Y ppm (AR)	Tot Y ppm	Zr ppm (AR)	Tot Zr ppm	Mo ppm (AR)	Tot Mo ppm
96018-001	11	16	30	6.7	6.9	1.5	11	25	34
96018-002	12	135	147	39	42	15	55	127	137
96018-003	10	32	45	9.4	9	2.8	13	42	39
96018-004	9	147	157	31	32	12	46	100	108
96018-005	8	22	39	5.9	6.6	2.2	13	19	27
96018-006	3	160	176	27	28	9.9	41	46	52
96018-007	<3	27	39	5.2	6.1	1.8	12	11	15
96018-008	9	82	87	11	11	4.2	16	30	23
96018-009	6	193	217	23	25	8.5	40	35	41
96018-010	<3	75	91	11	12	4.3	23	31	36
96018-011	<3	251	237	8.5	8.6	4.0	6.2	2	4
96018-012	<3	381	386	15	14	3.7	9.3	4	7
96018-013	<3	84	98	9.1	9.5	2.7	11	5	6
96018-014	<3	317	319	11	11	2.3	7.6	6	8
96018-015	<3	177	204	14	14	7.0	29	23	26
96018-016	<3	260	275	13	13	4.9	19	8	9
96018-017	8	162	191	13	14	6.6	26	23	27
96018-018	6	254	267	26	26	5.8	24	20	23
96018-019	<3	113	118	15	15	4.1	22	4	5
96018-020	6	71	91.4	14	15	5.0	27	7	11
96018-021	<3	322	315	2.7	2.5	2.7	2.0	2	4
96018-022	23	222	241	27	28	11	63	13	17
96018-023	7	396	413	11	11	2.7	11	5	7
96018-024	<3	148	168	9.4	10	4.6	16	10	12
96018-026	9	331	335	14	14	7.0	22	8	11
96018-027	<3	414	447	11	12	4.9	15	5	8
96018-028	<3	100	109	3.1	3.2	1.6	8.3	2	4
96018-029	<3	339	366	12	13	6.7	22	6	9
96018-030	5	510	556	2.5	2.6	2.1	3.3	<1	2
96018-031	7	229	254	20	21	4.4	19	7	10
96018-032	9	158	190	11	12	3.6	15	8	11

Table A2. Continued.

Sample id	Ag ppm (AR)	Ba ppm (AR)	Tot Ba ppm	La ppm (AR)	Tot La ppm	Pb ppm (AR)	Tot Pb ppm
96018-001	0.3	12	86	3.5	3.9	76	91
96018-002	<2	17	106	21	23	38	34
96018-003	0.2	10	88	5.7	5.1	106	89
96018-004	0.5	13	105	17	19	36	33
96018-005	0.3	9	82	3.3	3.9	81	101
96018-006	0.2	9	97	15	17	35	32
96018-007	0.6	6	49	2.8	3.7	65	52
96018-008	0.2	11	84	6.8	6.5	142	97
96018-009	<2	9	96	13	15	29	27
96018-010	<2	10	90	6.5	7	121	109
96018-011	<2	2	3	5.2	2.8	6	3
96018-012	<2	6	20	11	8.5	6	<2
96018-013	0.3	8	20	5.2	4.5	4	<2
96018-014	0.3	5	17	6.7	5.6	6	<2
96018-015	<2	11	66	11	13	7	6
96018-016	0.3	7	43	9.5	9.2	5	<2
96018-017	0.3	10	62	11	12	10	8
96018-018	0.7	11	57	15	15	7	4
96018-019	0.2	6	27	8.4	7.5	5	<2
96018-020	0.3	5	41	7.6	7.9	6	4
96018-021	<2	3	1	3	0.7	<2	<2
96018-022	0.5	14	115	15	19	12	7
96018-023	<2	6	23	6.4	5.5	6	<2
96018-024	0.5	6	34	7	6.6	6	<2
96018-026	<2	9	36	13	13	8	3
96018-027	<2	8	26	11	10	5	<2
96018-028	0.3	5	16	3	2.4	3	2
96018-029	0.4	8	35	12	12	8	<2
96018-030	<2	2	4	2.5	1.2	3	<2
96018-031	0.6	9	43	11	11	6	<2
96018-032	0.3	9	36	6	5.9	4	3

Table A2. Continued.

Sample id	SIO2 % (calc)	Clay % (calc)	Calcite % (calc)
96018-001	92	2.3	1.1
96018-002	54	10	8.3
96018-003	88	2.5	2.2
96018-004	53	9.6	9.4
96018-005	91	2.4	1.7
96018-006	58	8.2	12
96018-007	92	2.0	1.9
96018-008	81	3.2	5.5
96018-009	59	8.9	12
96018-010	80	3.6	5.7
96018-011	21	0.82	38
96018-012	36	2.2	30
96018-013	86	1.6	6.2
96018-014	28	1.9	35
96018-015	61	5.2	10
96018-016	60	3.8	17
96018-017	62	5.3	9.5
96018-018	55	5.9	20
96018-019	78	2.4	9.7
96018-020	85	5.1	5.9
96018-021	18	0.19	40
96018-022	60	14	16
96018-023	44	2.4	27
96018-024	70	2.9	13
96018-026	39	3.9	21
96018-027	40	2.7	24
96018-028	85	1.2	5.5
96018-029	44	3.7	19
96018-030	28	0.58	35
96018-031	69	3.8	13
96018-032	77	2.6	8.6
			0.0

Table A2. Continued.

Sample id	Field no.	m above base	Locality	Age	Lithology	Color	T_{MAX} °C	S1 mg/gm	S2 mg/gm
96018-033	UK32	19.70	Outcrop 28	L. - M. Domanik	massive shale	brown	421	0.62	23
96018-034	UK33	20.00	Outcrop 28	L. - M. Domanik	massive shale	brown	418	4.3	42
96018-035	UK34	20.35	Outcrop 28	L. - M. Domanik	massive shale	brown	418	4.6	42
96018-036	UK35	20.40	Outcrop 28	L. - M. Domanik	massive shale	brown	420	1.7	18
96018-037	UK36	20.73	Outcrop 28	L. - M. Domanik	limestone	brown	423	0.02	0.81
96018-038	UK37	20.96	Outcrop 28	L. - M. Domanik	massive shale	brown	420	3.3	35
96018-039	UK38	21.26	Outcrop 28	L. - M. Domanik	massive shale	brown	419	1.6	26
96018-040	UK39	22.46	Outcrop 28	L. - M. Domanik	limestone	brown	425	0.1	2.3
96018-041	UK40	23.46	Outcrop 28	L. - M. Domanik	massive shale	brown	421	2.1	28
96018-042	UK41	20.60	Old Motor Road Q.	M. Domanik	limestone	brown	424	0.26	3
96018-043	UK42	20.16	Old Motor Road Q.	M. Domanik	massive shale	brown	418	2.2	25
96018-044	UK43	19.58	Old Motor Road Q.	M. Domanik	massive shale	brown	422	5.4	45
96018-045	UK44	18.95	Old Motor Road Q.	M. Domanik	massive shale	brown	421	6.4	44
96018-046	UK45	18.85	Old Motor Road Q.	M. Domanik	massive shale	brown	420	3.0	31
96018-047	UK46	22.27	Old Motor Road Q.	M. Domanik	massive shale	brown	421	1.8	23
96018-048	UK47	22.63	Old Motor Road Q.	M. Domanik	massive shale	brown	420	2.4	27
96018-049	UK48	24.25	Old Motor Road Q.	M. Domanik	massive shale	brown	419	2.2	26
96018-050	UK49	27.00	Yankee Q.	M. Domanik	limestone	brown	424	1.2	5.3
96018-051	UK50	27.82	Yankee Q.	M. Domanik	massive shale	brown	421	2.0	23
96018-052	UK51	36.53	Outcrop 21	M. - U. Domanik	massive shale	brown	421	3.5	22
96018-053	UK52	36.58	Outcrop 21	M. - U. Domanik	massive shale	brown	421	2.1	15
96018-054	UK53	36.80	Outcrop 21	M. - U. Domanik	massive shale	brown	419	3.9	32
96018-055	UK54	37.12	Outcrop 21	M. - U. Domanik	massive shale	brown	421	3.5	26
96018-056	UK55	37.22	Outcrop 21	M. - U. Domanik	massive shale	brown	421	3.6	26
96018-057	UK56	37.48	Outcrop 21	M. - U. Domanik	massive shale	brown	422	3.8	32
96018-058	UK57	37.54	Outcrop 21	M. - U. Domanik	massive shale	brown	421	4.4	34
96018-059	UK58	38.01	Outcrop 21	M. - U. Domanik	massive shale	brown	421	2.0	17
96018-060	UK59	38.25	Outcrop 21	M. - U. Domanik	massive shale	brown	420	3.1	29
96018-061	UK60	38.65	Outcrop 21	M. - U. Domanik	massive shale	brown	420	2.9	27
96018-062	UK61	38.76	Outcrop 21	M. - U. Domanik	massive shale	brown	422	1.4	12
96018-063	UK62 (P-94)	39.55	Outcrop 21	M. - U. Domanik	massive shale	brown	422	2.9	38
96018-064	UK63	39.59	Outcrop 21	M. - U. Domanik	massive shale	brown	424	0.61	6.7
96018-065	UK64	40.14	Outcrop 21	M. - U. Domanik	massive shale	brown	419	3.9	31

Table A2. Continued.

Sample id	S3 mg/gm	PI	S2/S3	PC	TOC %	HI	OI	Total S %	Na % (AR)	Tot Na %	Mg % (AR)	Tot Mg %
96018-033	0.83	0.03	27	1.9	4.4	509	18	0.98	0.03	0.06	0.15	0.45
96018-034	0.94	0.09	45	3.9	7.1	592	13	0.74	0.02	0.05	0.08	0.14
96018-035	2.0	0.10	21	3.8	8.9	465	22	0.65	0.03	0.04	0.22	0.30
96018-036	0.84	0.08	22	1.7	3.2	579	26	0.33	0.02	0.05	0.09	0.12
96018-037	0.17	0.02	4.8	0.06	0.21	385	80	0.001	0.02	0.02	0.31	0.37
96018-038	0.98	0.09	35	3.2	6.4	545	15	0.80	0.02	0.06	0.10	0.15
96018-039	0.89	0.06	29	2.3	4.4	597	20	0.44	0.02	0.06	0.06	0.10
96018-040	0.22	0.04	10	0.2	0.47	489	46	0.14	0.02	0.03	0.31	0.35
96018-041	2.1	0.07	13	2.5	5.8	481	36	0.55	0.03	0.05	0.13	0.23
96018-042	0.48	0.08	6.3	0.27	0.67	447	71	0.067	0.02	0.03	0.69	0.76
96018-043	1.3	0.08	19	2.3	4.4	570	30	0.35	0.02	0.07	0.03	0.09
96018-044	3.04	0.11	15	4.2	9.4	483	32	0.67	0.03	0.05	0.37	0.26
96018-045	1.3	0.13	34	4.2	7.9	563	16	0.90	0.03	0.05	0.46	0.46
96018-046	0.93	0.09	33	2.8	5.0	613	18	0.41	0.02	0.07	0.05	0.11
96018-047	1.5	0.07	15	2.0	4.4	518	34	0.33	0.02	0.06	0.07	0.14
96018-048	1.7	0.08	15	2.4	5.0	532	34	0.32	0.03	0.07	0.07	0.15
96018-049	2.1	0.08	12	2.4	5.1	507	41	0.27	0.03	0.06	0.09	0.16
96018-050	0.8	0.18	6.6	0.54	1.2	438	66	0.11	0.02	0.04	0.28	0.31
96018-051	1.8	0.08	13	2.1	4.4	515	40	0.19	0.03	0.07	0.12	0.19
96018-052	0.29	0.14	75	2.1	3.6	600	8	0.52	0.02	0.05	0.06	0.10
96018-053	0.38	0.13	39	1.4	2.8	527	13	0.37	0.02	0.05	0.13	0.16
96018-054	1.1	0.11	31	3	6.1	528	17	0.59	0.03	0.05	0.15	0.21
96018-055	0.48	0.12	55	2.5	4.4	600	10	0.56	0.02	0.06	0.06	0.10
96018-056	0.39	0.12	67	2.5	4.4	592	8	0.59	0.02	0.05	0.07	0.11
96018-057	0.55	0.1	59	3.0	5.4	604	10	0.64	0.02	0.05	0.14	0.21
96018-058	0.71	0.12	47	3.2	6.0	558	11	0.83	0.02	0.06	0.26	0.36
96018-059	0.73	0.10	24	1.6	3.3	529	22	0.49	0.02	0.05	0.35	0.43
96018-060	1.1	0.10	26	2.7	5.3	556	21	0.69	0.02	0.05	0.49	0.58
96018-061	1.1	0.10	25	2.5	4.8	557	22	0.51	0.03	0.05	1.57	1.6
96018-062	0.73	0.10	16	1.1	2.4	494	31	0.30	0.02	0.05	0.08	0.09
96018-063	2.4	0.07	16	3.4	7.8	487	30	0.61	0.02	0.05	0.09	0.15
96018-064	0.68	0.08	9.8	0.6	1.5	443	45	0.19	0.02	0.05	0.02	0.03
96018-065	1.3	0.11	25	2.9	5.9	525	21	0.58	0.02	0.06	0.23	0.36

Table A2. Continued.

Sample id	Al % (AR)	Tot Al%	P% (AR)	Tot P %	K% (AR)	Tot K %	Ca % (AR)	Tot Ca %	Sc ppm (AR)	Tot Sc ppm	Tot Ti %
96018-033	0.16	2.9	0.05	0.05	0.11	1.0	11	12	2.4	5.1	0.19
96018-034	0.03	0.53	0.03	0.03	0.03	0.20	7.2	9.2	1.1	1.5	0.03
96018-035	0.06	0.77	0.04	0.05	0.05	0.29	19	21	2.0	2.7	0.04
96018-036	0.03	0.45	0.02	0.02	0.03	0.16	8.7	9.8	0.8	1.0	0.02
96018-037	<0.01	0.18	<0.01	0.01	<0.01	0.02	29	38	<0.5	0.6	<0.01
96018-038	0.03	0.59	0.03	0.04	0.03	0.21	8.8	10	1.3	1.5	0.03
96018-039	0.03	0.45	0.02	0.03	0.02	0.15	5.5	6.6	0.8	1.0	0.01
96018-040	0.02	0.19	0.02	0.02	0.02	0.08	29	33	<0.5	0.9	0.01
96018-041	0.05	0.81	0.06	0.06	0.05	0.33	12	14	1.5	2.2	0.04
96018-042	0.02	0.25	0.03	0.03	0.02	0.10	27	31	0.6	1.0	0.01
96018-043	0.04	0.64	0.04	0.04	0.03	0.21	2.9	3.4	0.7	1.2	0.03
96018-044	0.06	0.80	0.12	0.12	0.05	0.30	13	15	2.1	2.7	0.04
96018-045	0.06	0.89	0.06	0.06	0.05	0.33	11	13	1.9	2.8	0.04
96018-046	0.04	0.63	0.04	0.05	0.03	0.18	5.1	6.3	1.0	1.3	0.02
96018-047	0.04	0.63	0.03	0.04	0.03	0.22	7.9	9.9	0.8	1.3	0.03
96018-048	0.05	0.89	0.05	0.05	0.04	0.30	7.0	8.3	1.2	1.9	0.04
96018-049	0.04	0.79	0.04	0.05	0.04	0.26	8.5	11	1.0	1.8	0.03
96018-050	0.02	0.26	0.02	0.02	0.02	0.09	25	30	0.5	0.8	0.01
96018-051	0.07	0.80	0.04	0.05	0.04	0.28	10	12	1.5	1.9	0.04
96018-052	0.04	0.45	0.04	0.05	0.03	0.15	5.3	6.8	0.7	1.1	0.02
96018-053	0.03	0.37	0.03	0.04	0.02	0.13	10	12	0.7	1.0	0.02
96018-054	0.06	0.62	0.05	0.05	0.04	0.22	13	15	1.3	1.7	0.03
96018-055	0.04	0.53	0.04	0.05	0.03	0.16	5.5	7.0	0.8	1.4	0.02
96018-056	0.04	0.52	0.06	0.06	0.03	0.17	7.2	8.1	1.1	1.4	0.02
96018-057	0.06	0.75	0.09	0.09	0.04	0.26	8.1	9.2	1.5	2.0	0.03
96018-058	0.07	0.88	0.10	0.11	0.05	0.32	8.5	11	1.5	2.4	0.04
96018-059	0.07	0.75	0.06	0.06	0.04	0.26	14	16	1.7	2.3	0.04
96018-060	0.05	0.77	0.05	0.06	0.04	0.26	8.7	11	1.3	2.1	0.03
96018-061	0.05	0.52	0.04	0.04	0.04	0.18	15	17	1.5	1.8	0.03
96018-062	0.03	0.33	0.02	0.02	0.02	0.10	2.1	2.5	0.6	0.6	0.01
96018-063	0.05	0.63	0.08	0.07	0.04	0.23	8.9	10	1.7	1.9	0.03
96018-064	0.03	0.24	0.03	0.03	0.02	0.08	1.6	2.0	<0.5	<0.5	<0.01
96018-065	0.09	1.3	0.07	0.07	0.06	0.46	7.9	9.7	1.8	2.7	0.06

Table A2. Continued.

Sample id	V ppm (AR)	Tot V ppm	Cr ppm (AR)	Tot Cr ppm	Mn ppm (AR)	Tot Mn ppm	Fe % (AR)	Tot Fe %	Co ppm (AR)
96018-033	67	210	5	40	140	146	0.71	1.07	3
96018-034	172	280	4	13	62	68	0.19	0.26	3
96018-035	453	658	9	29	106	103	0.22	0.29	2
96018-036	171	251	4	12	73	72	0.24	0.22	1
96018-037	38	57	<1	<1	118	127	0.07	0.08	<1
96018-038	322	441	5	21	38	42	0.35	0.39	<1
96018-039	237	317	3	14	31	33	0.12	0.16	2
96018-040	28	38	2	2	67	67	0.09	0.11	2
96018-041	434	708	9	33	34	40	0.25	0.33	2
96018-042	37	52	4	7	79	79	0.12	0.15	<1
96018-043	190	346	4	22	12	14	0.17	0.23	<1
96018-044	586	946	19	54	31	37	0.29	0.38	2
96018-045	302	461	9	29	34	37	0.27	0.36	2
96018-046	203	352	5	24	23	29	0.19	0.24	<1
96018-047	144	276	3	12	26	31	0.18	0.25	1
96018-048	186	391	5	25	31	34	0.19	0.28	2
96018-049	73	175	4	13	64	69	0.33	0.43	2
96018-050	74	121	4	5	82	78	0.20	0.22	<1
96018-051	128	419	6	23	58	61	0.21	0.30	2
96018-052	217	346	6	22	16	20	0.16	0.21	1
96018-053	225	310	9	18	25	27	0.09	0.12	1
96018-054	392	578	9	28	37	40	0.13	0.19	<1
96018-055	245	390	6	23	30	34	0.19	0.26	2
96018-056	277	404	8	25	28	30	0.15	0.18	<1
96018-057	305	483	7	28	27	30	0.15	0.22	3
96018-058	342	571	8	31	30	35	0.32	0.45	2
96018-059	192	308	8	25	73	78	0.21	0.31	3
96018-060	222	313	5	15	53	56	0.26	0.39	2
96018-061	271	324	9	17	58	57	0.12	0.17	<1
96018-062	110	129	3	8	8	8	0.07	0.08	1
96018-063	415	621	15	44	22	24	0.14	0.19	1
96018-064	141	176	6	13	4	5	0.07	0.09	<1
96018-065	282	540	7	33	37	40	0.24	0.37	<1

Table A2. Continued.

Sample id	Tot Co ppm	Ni ppm (AR)	Tot Ni ppm	Cu ppm (AR)	Tot Cu ppm	Zn ppm (AR)	Tot Zn ppm	As ppm (AR)
96018-033	3	65	65	41	38	45	49	5
96018-034	2	100	114	39	39	27	28	5
96018-035	1	93	91	56	50	191	172	3
96018-036	1	38	40	24	20	96	85	5
96018-037	<1	5	5	4.7	<0.5	14	11	5
96018-038	1	53	55	43	38	109	104	8
96018-039	2	40	42	23	19	68	69	6
96018-040	<1	8	9	7.5	<0.5	27	23	4
96018-041	2	85	90	40	37	156	157	9
96018-042	<1	14	14	8.9	3.4	35	31	3
96018-043	<1	42	43	22	20	59	60	<3
96018-044	<1	106	103	65	63	170	159	10
96018-045	1	99	92	67	56	162	145	9
96018-046	1	41	62	27	30	108	115	4
96018-047	<1	37	40	22	20	41	42	6
96018-048	1	56	59	34	30	100	100	6
96018-049	2	46	49	29	27	26	26	9
96018-050	<1	20	19	9.1	2.7	37	30	3
96018-051	<1	63	65	27	24	49	48	<3
96018-052	1	39	46	26	25	132	150	<3
96018-053	1	39	40	21	18	98	95	<3
96018-054	<1	49	50	36	31	65	60	8
96018-055	1	38	42	30	29	82	87	8
96018-056	<1	42	42	31	26	87	83	5
96018-057	<1	51	51	35	33	81	80	5
96018-058	1	62	68	38	37	116	125	7
96018-059	1	36	38	28	25	80	79	6
96018-060	2	50	55	28	27	76	79	7
96018-061	<1	43	44	32	28	65	63	5
96018-062	<1	23	23	16	14	22	22	5
96018-063	<1	90	86	44	37	139	128	6
96018-064	1	29	36	15	14	41	43	<3
96018-065	1	53	56	33	30	80	79	4

Table A2. Continued.

Sample id	Tot As ppm	Sr ppm (AR)	Tot Sr ppm	Y ppm (AR)	Tot Y ppm	Zr ppm (AR)	Tot Zr ppm	Mo ppm (AR)	Tot Mo ppm
96018-033	7	227	250	17	19	12	99	13	17
96018-034	4	122	174	14	16	3.7	18	48	58
96018-035	5	323	345	33	32	7.2	23	21	25
96018-036	<3	129	186	13	12	4.3	14	7	10
96018-037	8	338	371	4.6	4.9	4.2	4.3	3	4
96018-038	<3	154	229	18	18	5.7	21	16	16
96018-039	8	107	182	10	10	3.9	15	7	10
96018-040	10	658	653	9.0	8.9	3.5	5.3	1	4
96018-041	9	238	305	23	24	6.5	23	9	12
96018-042	<3	422	416	9.9	9.4	2.9	5.7	2	4
96018-043	<3	64	112	10	11	2.6	18	5	8
96018-044	8	281	309	32	31	8.6	26	16	18
96018-045	6	224	276	22	21	7.2	25	46	48
96018-046	<3	108	157	14	14	3.6	14	9	11
96018-047	10	248	312	11	12	3.9	18	8	10
96018-048	11	205	242	16	16	3.5	20	7	9
96018-049	12	325	535	12	13	3.1	17	12	14
96018-050	<3	932	937	9.5	9.3	3.4	6.2	2	4
96018-051	5	391	425	18	19	4.0	20	4	5
96018-052	7	120	154	12	14	3.8	13	6	8
96018-053	<3	225	235	11	12	3.5	11	6	7
96018-054	5	304	324	20	20	5.5	17	8	10
96018-055	13	132	168	13	13	2.7	13	5	6
96018-056	6	186	199	16	16	3.7	14	6	7
96018-057	4	208	225	21	21	4.4	18	8	9
96018-058	8	222	263	22	24	5.5	21	11	15
96018-059	8	362	392	20	20	4.3	17	6	9
96018-060	11	207	257	16	16	5.2	18	16	20
96018-061	<3	361	377	16	16	5.7	16	12	13
96018-062	8	58	75	6.2	6.0	3.0	11	6	7
96018-063	7	207	220	24	23	6.1	20	7	8
96018-064	8	50	65	7.3	6.9	2.5	9.4	3	3
96018-065	11	217	265	20	21	5.2	25	14	17

Table A2. Continued.

Sample id	Ag ppm (AR)	Ba ppm (AR)	Tot Ba ppm	La ppm (AR)	Tot La ppm	Pb ppm (AR)	Tot Pb ppm
96018-033	0.6	11	93	14	23	6	3
96018-034	0.5	5	35	8.1	9.2	7	<2
96018-035	0.4	7	31	19	18	4	<2
96018-036	<2	5	22	7.3	6.7	6	4
96018-037	<2	2	1	3	1.1	4	<2
96018-038	0.9	5	26	10	11	8	4
96018-039	0.4	5	26	5.8	6	7	3
96018-040	0.3	4	9	6.3	4.3	3	<2
96018-041	0.9	7	44	10	11	8	3
96018-042	0.3	4	11	6.6	4.9	5	<2
96018-043	0.3	11	44	4.8	6.0	6	2
96018-044	0.9	10	41	15	14	8	4
96018-045	0.6	8	42	11	12	9	5
96018-046	0.5	7	36	6.3	6.8	5	<2
96018-047	<2	8	39	5.8	6.6	4	<2
96018-048	0.4	9	52	8.6	8.6	<2	<2
96018-049	0.4	8	57	6	7.4	3	<2
96018-050	0.2	12	22	6.2	4.5	7	<2
96018-051	0.4	11	69	12	11	4	<2
96018-052	0.6	5	20	5.9	6.1	7	<2
96018-053	0.6	4	17	5.7	5.2	2	<2
96018-054	0.5	7	28	9.6	9.5	8	<2
96018-055	0.7	4	22	5.3	6.0	5	2
96018-056	0.5	5	24	7.8	7.0	5	<2
96018-057	<2	6	35	9.8	10	4	<2
96018-058	0.5	6	40	11	12	4	4
96018-059	<2	6	32	11	11	4	4
96018-060	0.6	6	38	8.1	9.2	5	4
96018-061	0.4	5	22	9.6	8.8	8	3
96018-062	0.6	5	18	3.2	3.0	4	2
96018-063	0.7	6	29	11	10	7	4
96018-064	0.6	4	14	3.3	3.1	5	6
96018-065	0.5	8	53	10	12	5	4

Table A2. Continued.

Sample id	SIO2 % (calc)	Clay % (calc)	Calcite % (calc)
96018-033	68	14	14
96018-034	73	2.5	9.1
96018-035	42	3.7	23
96018-036	74	2.2	11
96018-037	25	0.86	37
96018-038	70	2.8	11
96018-039	81	2.2	6.9
96018-040	26	0.91	36
96018-041	63	3.9	15
96018-042	29	1.2	34
96018-043	87	3.1	3.8
96018-044	54	3.8	17
96018-045	61	4.3	14
96018-046	81	3.0	6.5
96018-047	75	3.0	10
96018-048	76	4.3	8.9
96018-049	72	3.8	11
96018-050	34	1.2	32
96018-051	68	3.8	13
96018-052	82	2.2	6.7
96018-053	70	1.8	13
96018-054	60	3.0	16
96018-055	81	2.5	7.0
96018-056	77	2.5	9.1
96018-057	73	3.6	10
96018-058	70	4.2	11
96018-059	60	3.6	18
96018-060	70	3.7	11
96018-061	52	2.5	19
96018-062	92	1.6	2.8
96018-063	68	3.0	11
96018-064	94	1.2	2.1
96018-065	72	6.1	10

Table A2. Continued.

Sample id	Field no.	m above base	Locality	Age	Lithology	Color	T_{MAX} °C	S1 mg/gm	S2 mg/gm
96018-066	UK65 (P-96)	41.00	Outcrop 21	M. - U. Domanik	massive shale	brown	420	3.3	28
96018-067	UK66	41.20	Outcrop 21	M. - U. Domanik	massive shale	brown	424	4.1	39
96018-068	UK67	41.55	Outcrop 21	M. - U. Domanik	massive shale	brown	418	4.8	38
96018-069	UK68	41.78	Outcrop 21	M. - U. Domanik	limestone	brown	424	0.1	1.4
96018-070	UK69	42.03	Outcrop 21	M. - U. Domanik	fissile shale	black	422	5.1	63
96018-071	UK70	43.42	Outcrop 21	M. - U. Domanik	fissile shale	brown	422	2.9	36
96018-072	UK71	43.50	Outcrop 21	M. - U. Domanik	limestone	brown	415	0.64	2.8
96018-073	UK72	43.58	Outcrop 21	M. - U. Domanik	massive shale	brown	416	4.4	41
96018-074	UK73	44.42	Outcrop 21	M. - U. Domanik	limestone	brown	424	0.06	1.0
96018-075	UK74	44.50	Outcrop 21	M. - U. Domanik	fissile shale	brown	424	1.9	26
96018-076	UK75	44.79	Black Dog Q.	M. - U. Domanik	massive shale	brown	416	2.3	23
96018-077	UK76	45.38	Black Dog Q.	M. - U. Domanik	massive shale	brown	420	2.5	26
96018-078	UK77	45.66	Black Dog Q.	M. - U. Domanik	massive shale	brown	419	4.4	39
96018-079	UK78	45.83	Black Dog Q.	M. - U. Domanik	massive shale	black	418	10	84
96018-080	UK79	45.85	Black Dog Q.	M. - U. Domanik	massive shale	brown	419	3.4	36
96018-081	UK80	46.49	Black Dog Q.	M. - U. Domanik	massive shale	brown	420	1.6	17
96018-082	UK81	47.45	Black Dog Q.	M. - U. Domanik	massive shale	brown	418	1.4	24
96018-083	UK82	47.76	Black Dog Q.	M. - U. Domanik	massive shale	brown	420	1.9	17
96018-084	UK83	48.21	Black Dog Q.	M. - U. Domanik	limestone	brown	420	0.13	1.4
96018-085	UK84	48.47	Black Dog Q.	M. - U. Domanik	massive shale	brown	418	4.4	37
96018-086	UK85	48.57	Black Dog Q.	M. - U. Domanik	massive shale	brown	418	6.3	50
96018-087	UK86	49.17	Black Dog Q.	M. - U. Domanik	massive shale	brown	415	8.4	61
96018-088	UK87	49.63	Black Dog Q.	M. - U. Domanik	massive shale	brown	414	7.5	56
96018-089	UK88	50.25	Black Dog Q.	M. - U. Domanik	clay	brown	415	0.49	12
96018-090	UK89	51.19	Black Dog Q.	M. - U. Domanik	massive shale	black	417	6.1	44
96018-091	UK90	51.21	Black Dog Q.	M. - U. Domanik	nd	nd	418	4.0	24
96018-092	UK91	53.44	Black Dog Q.	M. - U. Domanik	massive shale	brown	423	1.6	22
96018-093	UK92	54.76	Black Dog Q.	M. - U. Domanik	limestone	brown	419	0.28	2.6
96018-094	UK93	55.17	Black Dog Q.	M. - U. Domanik	fissile shale	brown	423	1.2	16

Table A2. Continued.

Sample id	S3 mg/gm	PI	S2/S3	PC	TOC %	HI	OI	Total S %	Na % (AR)	Tot Na %	Mg % (AR)	Tot Mg %
96018-066	1.5	0.10	19	2.6	5.4	518	27	0.52	0.02	0.05	0.33	0.42
96018-067	3.5	0.10	11	3.6	8.9	434	39	0.84	0.02	0.06	0.08	0.25
96018-068	1.6	0.11	23	3.6	7.1	533	22	0.66	0.03	0.05	0.12	0.23
96018-069	0.38	0.07	3.7	0.12	0.42	330	90	0.20	0.02	0.02	0.27	0.28
96018-070	6.2	0.07	10	5.7	15	413	40	1.1	0.02	0.05	0.08	0.30
96018-071	2.7	0.08	13	3.2	6.7	534	40	0.45	0.02	0.05	0.08	0.17
96018-072	0.17	0.19	16	0.28	0.47	593	36	0.06	0.02	0.02	0.36	0.36
96018-073	1.3	0.10	32	3.8	6.8	602	19	0.60	0.03	0.04	0.15	0.20
96018-074	0.29	0.06	3.5	0.09	0.26	392	111	0.05	0.02	0.03	0.36	0.37
96018-075	2.6	0.07	10	2.3	5.5	475	46	0.34	0.03	0.06	0.16	0.32
96018-076	0.66	0.09	35	2.1	3.9	593	16	0.37	0.02	0.06	0.06	0.11
96018-077	1.7	0.09	16	2.4	5.2	503	32	0.45	0.02	0.05	0.14	0.25
96018-078	0.76	0.10	52	3.6	6.9	570	11	0.73	0.03	0.05	0.16	0.25
96018-079	1.4	0.11	61	7.8	16	515	8	1.6	0.02	0.05	0.08	0.29
96018-080	0.61	0.09	59	3.3	6.3	572	9	0.57	0.02	0.06	0.04	0.12
96018-081	0.85	0.08	20	1.5	3.1	540	27	0.31	0.03	0.05	3.4	3.4
96018-082	1.1	0.05	22	2.1	4.2	574	26	0.31	0.02	0.06	0.05	0.09
96018-083	0.79	0.10	21	1.6	3.1	547	25	0.32	0.02	0.06	0.04	0.07
96018-084	0.14	0.09	9.8	0.12	0.27	507	51	0.28	0.03	0.03	0.56	0.56
96018-085	0.80	0.11	46	3.4	6.3	579	12	0.60	0.03	0.05	0.91	1.0
96018-086	0.63	0.11	79	4.7	7.9	632	8	0.92	0.03	0.06	0.14	0.30
96018-087	1.9	0.12	32	5.8	12	518	16	1.3	0.03	0.06	0.09	0.30
96018-088	2.8	0.12	20	5.3	10	543	26	0.77	0.03	0.05	0.34	0.56
96018-089	0.33	0.04	37	1.1	2.5	493	13	4.5	0.02	0.37	0.10	0.87
96018-090	0.87	0.12	50	4.2	8.3	530	10	1.3	0.03	0.06	0.12	0.30
96018-091	0.64	0.14	38	2.3	4.2	575	15	0.43	0.03	0.06	0.18	0.22
96018-092	2.7	0.07	8.1	1.9	5.0	429	53	0.24	0.02	0.07	0.10	0.27
96018-093	0.31	0.10	8.3	0.23	0.70	365	44	1.1	0.02	0.03	0.29	0.33
96018-094	2.3	0.07	6.7	1.4	3.5	450	66	0.19	0.02	0.06	0.14	0.21

Table A2. Continued.

Sample id	Al % (AR)	Tot Al%	P% (AR)	Tot P %	K% (AR)	Tot K %	Ca % (AR)	Tot Ca %	Sc ppm (AR)	Tot Sc ppm	Tot Ti %
96018-066	0.07	0.84	0.07	0.07	0.05	0.31	13	15	1.6	2.3	0.04
96018-067	0.14	1.5	0.13	0.14	0.09	0.58	6.1	7.2	3.4	5.0	0.08
96018-068	<0.01	1.0	0.13	0.13	0.07	0.39	9.3	10	2.3	3.1	0.05
96018-069	0.01	0.12	0.02	0.02	<0.01	0.04	30	34	<0.5	1.1	<0.01
96018-070	0.16	1.9	0.15	0.17	0.10	0.71	5.7	6.9	2.6	4.9	0.09
96018-071	0.07	0.82	0.08	0.09	0.06	0.32	8.4	11	1.8	2.5	0.04
96018-072	<0.01	0.05	0.01	0.01	<0.01	0.02	31	35	<0.5	<0.5	<0.01
96018-073	0.05	0.52	0.08	0.08	0.04	0.19	17	20	1.1	1.5	0.03
96018-074	0.01	0.09	0.01	0.01	0.01	0.04	31	34	<0.5	0.8	<0.01
96018-075	0.11	1.5	0.08	0.10	0.07	0.53	11	15	2.0	3.5	0.09
96018-076	0.04	0.61	0.04	0.05	0.03	0.21	5.6	6.8	1.0	1.4	0.02
96018-077	<0.01	0.93	0.08	0.09	0.06	0.35	13	15	2.2	3.0	0.05
96018-078	0.09	0.94	0.08	0.09	0.06	0.35	14	16	1.7	2.8	0.04
96018-079	0.17	1.8	0.15	0.16	0.10	0.68	6.3	7.4	2.6	4.5	0.09
96018-080	0.06	0.82	0.05	0.06	0.05	0.27	3.9	5.0	1.2	1.9	0.03
96018-081	0.08	0.75	0.05	0.05	0.05	0.28	12	14	2.1	2.6	0.04
96018-082	0.04	0.51	0.05	0.05	0.03	0.16	5.0	6.2	0.9	1.2	0.02
96018-083	0.03	0.45	0.03	0.04	0.02	0.14	4.7	6.0	0.7	1.1	0.02
96018-084	0.02	0.13	0.01	0.01	0.01	0.03	31	34	<0.5	0.8	<0.01
96018-085	0.08	0.88	0.05	0.05	0.05	0.31	16	18	1.5	2.4	0.04
96018-086	0.13	1.5	0.09	0.10	0.08	0.55	9.4	11	1.9	3.3	0.08
96018-087	0.14	1.9	0.07	0.08	0.10	0.70	6.5	7.6	2.4	4.7	0.09
96018-088	0.08	0.99	0.06	0.07	0.06	0.38	15	18	1.3	2.4	0.04
96018-089	0.32	7.5	0.01	0.04	0.21	2.1	1.5	2.0	1.6	11	0.46
96018-090	0.14	2.4	0.05	0.05	0.09	0.61	8.6	9.7	1.8	3.6	0.11
96018-091	0.03	0.48	0.03	0.03	0.03	0.17	16	18	1.1	1.3	0.03
96018-092	0.11	1.5	0.05	0.06	0.08	0.53	8.3	10	2.0	3.4	0.10
96018-093	0.02	0.23	0.01	0.02	0.02	0.10	29	31	<0.5	0.8	0.01
96018-094	0.07	0.80	0.03	0.04	0.05	0.29	14	16	1.6	2.1	0.04

Table A2. Continued.

Sample id	V ppm (AR)	Tot V ppm	Cr ppm (AR)	Tot Cr ppm	Mn ppm (AR)	Tot Mn ppm	Fe % (AR)	Tot Fe %	Co ppm (AR)
96018-066	215	293	8	20	36	40	0.17	0.26	1
96018-067	579	1190	22	83	22	31	0.29	0.49	1
96018-068	467	810	18	54	33	37	0.27	0.37	2
96018-069	71	84	2	3	62	58	0.40	0.39	<1
96018-070	768	1770	25	94	18	36	0.27	0.53	1
96018-071	274	517	12	38	28	32	0.18	0.30	2
96018-072	21	21	1	<1	39	37	0.05	0.06	<1
96018-073	169	220	4	9	43	42	0.12	0.17	3
96018-074	61	65	2	1	100	95	0.10	0.10	<1
96018-075	184	438	11	39	55	67	0.29	0.48	2
96018-076	132	190	4	14	25	27	0.18	0.22	<1
96018-077	292	551	18	48	51	57	0.16	0.28	<1
96018-078	426	800	14	40	23	29	0.20	0.35	1
96018-079	920	1850	25	86	16	29	0.27	0.51	3
96018-080	345	717	9	35	13	17	0.21	0.29	1
96018-081	241	316	16	29	105	104	0.25	0.29	1
96018-082	183	300	6	20	386	407	0.12	0.16	<1
96018-083	145	221	4	11	17	21	0.10	0.14	<1
96018-084	40	46	1	1	48	44	0.24	0.24	<1
96018-085	202	291	7	17	63	65	0.24	0.32	2
96018-086	393	878	10	39	40	48	0.26	0.44	5
96018-087	423	925	10	44	35	44	0.65	0.83	4
96018-088	104	145	6	15	103	108	0.37	0.50	5
96018-089	30	191	9	85	74	95	3.3	4.0	20
96018-090	233	476	8	39	57	58	0.95	1.2	3
96018-091	129	182	5	11	77	74	0.14	0.20	2
96018-092	173	452	8	39	83	90	0.46	0.71	3
96018-093	39	79	2	4	113	108	0.92	0.81	2
96018-094	221	483	7	25	114	111	0.52	0.62	3

Table A2. Continued.

Sample id	Tot Co ppm	Ni ppm (AR)	Tot Ni ppm	Cu ppm (AR)	Tot Cu ppm	Zn ppm (AR)	Tot Zn ppm	As ppm (AR)
96018-066	<1	53	56	34	29	107	107	<3
96018-067	2	134	141	83	79	283	288	7
96018-068	1	81	80	54	46	163	154	7
96018-069	<1	16	16	7.8	1.0	78	70	7
96018-070	1	204	224	90	92	407	434	7
96018-071	1	82	91	48	48	115	120	6
96018-072	<1	6	6	3.4	<0.5	3.7	1.0	<3
96018-073	2	55	55	27	21	54	51	7
96018-074	<1	8	7	4.9	<0.5	19	15	<3
96018-075	2	82	90	54	55	169	180	4
96018-076	1	31	34	23	21	58	62	4
96018-077	1	71	74	35	32	136	138	4
96018-078	1	81	84	43	40	153	136	6
96018-079	3	219	224	89	87	402	416	9
96018-080	<1	64	68	38	36	120	125	9
96018-081	<1	47	48	32	28	113	111	6
96018-082	<1	85	90	22	19	101	104	4
96018-083	<1	35	38	19	18	39	40	<3
96018-084	<1	8	7	5.0	<0.5	25	21	4
96018-085	3	72	71	45	40	79	76	8
96018-086	3	150	156	57	56	216	218	7
96018-087	3	138	145	96	89	272	270	12
96018-088	5	68	66	38	34	40	40	6
96018-089	20	55	64	79	75	48	56	6
96018-090	3	144	138	73	63	259	242	21
96018-091	1	56	59	30	26	176	117	<3
96018-092	2	90	93	43	40	243	243	9
96018-093	<1	20	16	5.6	<0.5	9.5	9.2	6
96018-094	<1	65	63	30	26	277	262	11

Table A2. Continued.

Sample id	Tot As ppm	Sr ppm (AR)	Tot Sr ppm	Y ppm (AR)	Tot Y ppm	Zr ppm (AR)	Tot Zr ppm	Mo ppm (AR)	Tot Mo ppm
96018-066	<3	406	421	19	19	6.3	23	8	10
96018-067	8	209	265	40	41	11	43	15	18
96018-068	5	287	315	31	30	8.6	29	11	13
96018-069	4	480	468	8.7	8.1	1.2	2.8	7	7
96018-070	12	219	299	40	43	14	50	15	19
96018-071	8	265	349	21	23	7.2	27	7	10
96018-072	5	619	604	1.5	1.4	2.8	1.8	6	8
96018-073	19	507	526	18	17	4.8	15	37	40
96018-074	<3	905	853	7.1	6.5	3.4	3.5	2	3
96018-075	<3	516	623	23	26	6.9	39	4	6
96018-076	8	157	185	11	12	3.5	15	8	10
96018-077	3	400	454	27	28	6.3	25	6	8
96018-078	<3	357	397	23	24	6.0	23	22	27
96018-079	14	234	299	39	42	14	48	65	74
96018-080	10	137	212	16	17	5.0	20	23	27
96018-081	<3	352	376	16	16	5.0	18	8	12
96018-082	4	169	258	13	13	3.7	14	10	12
96018-083	6	149	203	9.3	10	3.7	13	14	17
96018-084	11	394	377	3.7	3.5	2.9	2.9	4	6
96018-085	13	544	594	20	20	5.2	21	43	47
96018-086	13	361	463	27	29	6.6	32	45	54
96018-087	12	263	365	21	23	12	47	56	66
96018-088	5	591	671	17	18	6.5	23	39	44
96018-089	8	48	246	3.9	17	22	319	2	4
96018-090	4	285	309	18	18	13	63	64	69
96018-091	6	470	490	13	13	6.6	21	29	35
96018-092	10	287	395	19	21	9.0	50	17	21
96018-093	<3	685	661	5.4	5.6	5.0	9	4	7
96018-094	7	486	612	32	31	6.5	26	25	27

Table A2. Continued.

Sample id	Ag ppm (AR)	Ba ppm (AR)	Tot Ba ppm	La ppm (AR)	Tot La ppm	Pb ppm (AR)	Tot Pb ppm
96018-066	0.4	7	45	9.9	10	8	4
96018-067	1.2	9	72	18	20	10	8
96018-068	1.0	7	44	15	15	8	3
96018-069	0.6	2	4	4.8	3.7	4	<2
96018-070	1.1	9	93	17	21	8	8
96018-071	0.5	5	37	10	12	6	4
96018-072	0.3	2	3	1.9	<0.5	-2	<2
96018-073	<2	5	28	9.9	9.2	5	<2
96018-074	<2	4	6	4.7	2.8	5	<2
96018-075	0.4	8	60	13	16	6	5
96018-076	0.2	5	27	5.8	6.5	4	4
96018-077	0.4	7	38	14	15	3	2
96018-078	1.0	6	43	11	12	6	3
96018-079	1.0	8	85	16	19	10	7
96018-080	1.0	5	38	6.7	8.2	7	5
96018-081	0.5	5	33	9.3	9.6	2	5
96018-082	0.3	7	26	6.0	7.0	3	<2
96018-083	<2	4	23	4.7	4.5	3	3
96018-084	<2	1	2	2.5	0.7	4	<2
96018-085	0.4	7	40	12	13	7	4
96018-086	0.7	8	69	12	15	8	6
96018-087	0.7	8	82	8.6	13	9	10
96018-088	0.3	7	50	10	12	4	5
96018-089	0.3	13	344	4.7	58	17	10
96018-090	2	8	72	10	15	10	8
96018-091	<2	5	31	8.4	8.2	6	<2
96018-092	0.5	11	65	11	15	7	4
96018-093	<2	5	11	3.3	1.9	6	<2
96018-094	1	12	45	15	16	<2	5

Table A2. Continued.

Sample id	SIO2 % (calc)	Clay % (calc)	Calcite % (calc)
96018-066	60	4.0	16
96018-067	74	7.3	8.1
96018-068	68	4.8	11.6
96018-069	24	0.58	37
96018-070	67	8.9	7.6
96018-071	71	3.9	11
96018-072	21	0.24	39
96018-073	48	2.5	22
96018-074	21	0.43	39
96018-075	64	7.2	15
96018-076	81	2.9	7.2
96018-077	62	4.5	16
96018-078	56	4.5	18
96018-079	65	8.4	8.4
96018-080	83	3.9	5.1
96018-081	54	3.6	15
96018-082	82	2.4	6.4
96018-083	84	2.2	6.0
96018-084	21	0.62	39
96018-085	49	4.2	20
96018-086	67	7.1	12
96018-087	69	9.1	8.6
96018-088	50	4.8	19
96018-089	93	36	2.9
96018-090	68	12	11
96018-091	54	2.3	20
96018-092	73	7.2	11
96018-093	26	1.1	36
96018-094	60	3.8	18

Table A3. Rock Eval data for finely spaced drill samples.

Sample id	Field no.	m above base	Sampling yr.	Locality	Age	T max °C	S1 mg/gm	S2 mg/gm
96019001	D1	22.18	1995	Old Motor Road Q.	M. Domanik	499	0.50	3.5
96019002	D2	22.22	1995	Old Motor Road Q.	M. Domanik	420	2.8	32
96019003	D3	22.28	1995	Old Motor Road Q.	M. Domanik	422	1.3	25
96019004	D4	22.35	1995	Old Motor Road Q.	M. Domanik	422	1.7	23
96019005	D5	22.65	1995	Old Motor Road Q.	M. Domanik	422	2.6	24
96019006	D6	22.81	1995	Old Motor Road Q.	M. Domanik	420	2.7	27
96019007	D7	22.87	1995	Old Motor Road Q.	M. Domanik	424	1.9	17
96019008	D8	23.18	1995	Old Motor Road Q.	M. Domanik	419	2.9	33
96019009	D9	23.25	1995	Old Motor Road Q.	M. Domanik	420	2.9	35
96019010	D10	23.49	1995	Old Motor Road Q.	M. Domanik	419	4.7	42
96019011	D11	45.34	1995	Black Dog Q.	M. - U. Domanik	419	5.8	45
96019012	D12	45.83	1995	Black Dog Q.	M. - U. Domanik	416	12	91
96019013	D13	45.85	1995	Black Dog Q.	M. - U. Domanik	419	3.5	32

Sample id	Field no.	S3 mg/gm	PI	S2/S3	PC	TOC	HI	OI
96019001	D1	4.0	0.12	0.87	0.33	0.33	1060	1212
96019002	D2	2.5	0.08	13	2.9	6.5	491	38
96019003	D3	1.9	0.05	14	2.2	5.0	511	37
96019004	D4	1.8	0.07	13	2.1	4.4	529	40
96019005	D5	1.9	0.10	12	2.2	4.8	502	40
96019006	D6	2.4	0.09	11	2.5	6.0	453	40
96019007	D7	2.4	0.10	7.1	1.6	3.9	430	60
96019008	D8	2.9	0.08	12	3.0	7.2	466	40
96019009	D9	2.8	0.08	13	3.2	7.4	474	37
96019010	D10	3.6	0.10	12	3.9	8.8	480	40
96019011	D11	1.3	0.11	35	4.2	8.4	535	15
96019012	D12	1.6	0.11	59	8.6	18	502	8
96019013	D13	0.79	0.10	40	2.9	6.0	528	13

Table A4. Information on samples in subset. All samples were collected in 1995.

Sample id	Field no.	m above base	Locality	Age	Lithology	Color
96018-001	UK1	0.12	Outcrop 7	L. Domanik	massive shale	brown
96018-002	UK2	0.16	Outcrop 7	L. Domanik	fissile shale	black
96018-003	UK3	0.20	Outcrop 7	L. Domanik	massive shale	brown
96018-004	UK4	0.22	Outcrop 7	L. Domanik	fissile shale	gray
96018-005	UK5	0.28	Outcrop 7	L. Domanik	massive shale	brown
96018-006	UK6	0.32	Outcrop 7	L. Domanik	fissile shale	black
96018-007	UK7	0.35	Outcrop 7	L. Domanik	massive shale	brown
96018-008	UK8	0.39	Outcrop 7	L. Domanik	massive shale	brown
96018-009	UK9	0.42	Outcrop 7	L. Domanik	fissile shale	gray
96018-010	UK10	0.45	Outcrop 7	L. Domanik	massive shale	brown
96018-011	UK11	0.57	Outcrop 7	L. Domanik	limestone	brown
96018-012	UK12	3.90	Outcrop 7	L. Domanik	limestone	brown
96018-016	UK16	9.80	Outcrop 7	L. Domanik	massive shale	brown
96018-017	UK17	9.85	Outcrop 7	L. Domanik	fissile shale	black
96018-028	UK28	15.25	Outcrop 7	L. Domanik	massive shale	black
96018-029	UK29	15.45	Outcrop 7	L. Domanik	massive shale	brown
96018-030	UK30	15.70	Outcrop 7	L. Domanik	limestone	brown
96018-031	UK31A	20.67	Outcrop 7	L. Domanik	massive shale	brown
96018-034	UK33	20.00	Outcrop 28	L. - M. Domanik	massive shale	brown
96018-035	UK34	20.35	Outcrop 28	L. - M. Domanik	massive shale	brown
96018-036	UK35	20.45	Outcrop 28	L. - M. Domanik	massive shale	brown
96018-037	UK36	20.73	Outcrop 28	L. - M. Domanik	limestone	brown
96018-044	UK43	19.58	Old Motor Road Q.	M. Domanik	massive shale	brown
96018-053	UK52	36.58	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-054	UK53	36.80	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-055	UK54	37.12	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-056	UK55	37.22	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-058	UK57	37.54	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-059	UK58	38.01	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-063	UK62	39.55	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-066	UK65	41.00	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-067	UK66	41.20	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-070	UK69	42.03	Outcrop 21	M. - U. Domanik	fissile shale	black
96018-071	UK70	43.42	Outcrop 21	M. - U. Domanik	fissile shale	brown
96018-072	UK71	43.50	Outcrop 21	M. - U. Domanik	limestone	brown
96018-073	UK72	43.58	Outcrop 21	M. - U. Domanik	massive shale	brown
96018-076	UK75	44.79	Black Dog Q.	M. - U. Domanik	massive shale	brown
96018-079	UK78	45.83	Black Dog Q.	M. - U. Domanik	massive shale	black
96018-086	UK85	48.57	Black Dog Q.	M. - U. Domanik	massive shale	brown
96018-088	UK87	49.63	Black Dog Q.	M. - U. Domanik	massive shale	brown
96018-089	UK88	50.25	Black Dog Q.	M. - U. Domanik	clay	brown
96018-092	UK91	53.44	Black Dog Q.	M. - U. Domanik	massive shale	brown
96018-093	UK92	54.76	Black Dog Q.	M. - U. Domanik	limestone	brown
96018-094	UK93	55.17	Black Dog Q.	M. - U. Domanik	fissile shale	brown

Table A5. Data on subset of sample, including mineralogy of the whole rock; atomic ratios of organic matter; carbon isotopes and V and Ni porphyrin (P) content in bitumen extracts; and sulfur speciation and their isotopic composition. Mineralogy in peak height (chart units), carbon isotope data relative to PDB standard, and sulfur isotopes relative to Cañon Diablo Troilite standard.

Sample id	m above base	Quartz pk ht	Calcite pk ht	atomic H/C	atomic O/C	atomic N/C	Bit. Ex. ppm	VP in bit	NiP in bit
96018-001	0.12	6302	69	1.17	0.109	0.029	15421	937	78
96018-002	0.16	1181	560	1.18	0.089	0.032	28548	1622	251
96018-003	0.20	5252	160	1.18	0.112	0.029	27576	834	73
96018-004	0.22	1364	124	1.16	0.078	0.033	26962	2758	372
96018-005	0.28	5907	178	1.18	0.064	0.031	24547	1581	98
96018-006	0.32	2259	1153	1.17	0.077	0.033	23235	2998	207
96018-007	0.35	5427	307	1.19	0.055	0.035	10105	2130	142
96018-008	0.39	4327	565	1.21	0.075	0.034	25492	1977	136
96018-009	0.42	2120	1196	1.19	0.069	0.032	21947	3028	228
96018-010	0.45	3883	582	1.19	0.091	0.031	23777	2175	132
96018-011	0.57	79	2701	1.13	0.124	0.033	1188	1467	111
96018-012	3.90	875	1771	1.20	0.054	0.030	7944	5080	215
96018-016	9.80	2325	1559	1.20	0.118	0.027	8577	583	38
96018-017	9.85	2658	912	1.20	0.080	0.028	14562	1065	114
96018-028	15.25	3870	694	1.23	0.068	0.028	5026	657	114
96018-029	15.45	1085	1597	1.23	0.070	0.028	23279	511	94
96018-030	15.70	156	2400	1.13	0.109	0.024	1606	67	15
96018-031	20.67	2066	786	1.20	0.119	0.025	5501	1445	84
96018-034	20.00	2965	786	1.24	0.068	0.029	15784	2906	392
96018-035	20.35	1009	1463	1.20	0.083	0.029	10234	6038	358
96018-036	20.40	3567	1121	1.22	0.079	0.028	14039	2495	78
96018-037	20.73	21	2979	nd	nd	nd	313	nd	nd
96018-044	19.58	1839	1299	1.18	0.105	0.031	22244	1213	80
96018-053	36.58	2403	884	1.22	0.052	0.030	5634	6037	254
96018-054	36.80	2812	1410	1.20	0.079	0.029	13692	2978	136
96018-055	37.12	2816	412	1.23	0.051	0.029	19833	2488	70
96018-056	37.22	3830	927	1.24	0.063	0.029	15970	2690	129
96018-058	37.54	3539	985	1.24	0.050	0.027	15359	2630	159
96018-059	38.01	1784	1270	1.22	0.066	0.029	5476	1005	76
96018-063	39.55	3329	1018	1.18	0.112	0.028	14399	1451	45

Table A5. Continued.

Sample id	$\delta^{13}C_{saturates}$	$\delta^{13}C_{aromatics}$	$\delta^{13}C_{kerogen}$	$S_{disulfide}$ wt%	$S_{organic}$ wt%	$\delta^{34}S_{disulfide}$	$\delta^{34}S_{organic}$
96018-001	-29.8	-29.2	-26.8	0.062	0.30	24.3	13.1
96018-002	-29.7	-28.2	-27.0	0.28	1.2	13.4	16.8
96018-003	-29.7	-29.2	-27.3	0.054	0.36	23.2	14.9
96018-004	-29.7	-28.2	-27.0	0.69	0.99	5.4	17.4
96018-005	-29.7	-29.7	-27.2	0.85	0.27	14.4	14.4
96018-006	-29.7	-28.5	-27.1	0.28	0.71	4.5	16.8
96018-007	-29.7	-29.0	-27.2	0.88	0.35	15.0	14.7
96018-008	-29.6	-29.1	-27.2	0.28	0.35	9.8	15.1
96018-009	-29.7	-28.6	-27.2	0.28	0.62	-2.9	15.7
96018-010	-29.6	-29.1	-26.9	0.12	0.38	7.9	14.3
96018-011	-29.6	-29.2	-27.2	0.084	0.044	10.4	insuff
96018-012	-30.0	-28.8	-28.6	0.082	0.22	4.2	12.6
96018-016	-29.6	-28.8	-29.5	0.0041	0.22	insuff	15.0
96018-017	-29.5	-27.9	-28.7	0.28	0.78	-4.3	18.5
96018-028	-29.7	-28.4	-28.3	0.52	0.33	14.0	17.4
96018-029	-29.7	-28.3	-28.2	0.39	0.77	-2.2	21.1
96018-030	-29.8	-28.9	-28.2	0.27	0.12	17.9	17.4
96018-031	-29.9	-29.3	-29.5	0.027	0.32	11.7	17.8
96018-034	-29.7	-28.2	-27.7	0.16	0.37	7.3	14.8
96018-035	-29.7	-27.9	-28.4	0.074	0.43	0.6	14.9
96018-036	-29.6	-28.5	-28.1	0.10	0.23	12.8	13.5
96018-037	-29.5	-27.9	nd	nd	nd	nd	nd
96018-044	-29.5	-29.1	-29.5	0.049	0.55	9.0	12.4
96018-053	-29.4	-29.0	-29.9	0.055	0.23	11.5	20.4
96018-054	-29.6	-29.1	-29.5	0.023	0.38	11.0	20.8
96018-055	-29.6	-29.2	-29.5	0.14	0.35	18.5	19.5
96018-056	-29.5	-29.2	-29.9	0.10	0.34	13.6	20.0
96018-058	-29.4	-29.1	-29.7	0.20	0.42	17.2	21.7
96018-059	-29.5	-28.9	-29.7	0.092	0.26	18.2	21.1
96018-063	-29.5	-29.2	-29.9	0.016	0.41	insuff	19.7

Table A5. Continued.

Sample id	m above base	Quartz pk ht	Calcite pk ht	atomic H/C	atomic O/C	atomic N/C	Bit. Ex. Ppm	VOP in bit	NiP in bit
96018-066	41.00	2485	1325	1.16	0.096	0.027	13158	1735	95
96018-070	42.03	2142	577	1.11	1.39	0.035	13926	947	30
96018-071	43.42	2960	1048	1.19	0.119	0.030	12202	1211	68
96018-072	43.50	134	3227	1.23	0.054	0.028	2688	1652	126
96018-073	43.58	1640	1799	1.21	0.071	0.023	13227	1344	58
96018-076	44.79	4477	731	1.21	0.062	0.027	11594	2443	118
96018-079	45.83	2386	758	1.19	0.064	0.034	19457	6633	485
96018-086	48.57	2593	1106	1.23	0.051	0.036	14698	3218	303
96018-088	49.63	1246	1731	1.19	1.01	0.030	14371	676	89
96018-089	50.25	1284	103	1.18	0.084	0.027	1849	939	145
96018-092	53.44	2880	1020	1.14	0.153	0.034	5451	328	66
96018-093	54.76	184	2998	1.19	0.072	0.036	840	4431	1814
96018-094	55.17	2381	1549	1.13	0.149	0.035	6197	589	48

Table A5. Continued.

Sample id	$\delta^{13}C_{saturates}$	$\delta^{13}C_{aromatics}$	$\delta^{13}C_{kerogen}$	$S_{disulfide}$ wt%	$S_{organic}$ wt%	$\delta^{34}S_{disulfide}$	$\delta^{34}S_{organic}$
96018-066	-29.5	-29.0	-29.6	0.033	0.36	10.2	17.8
96018-070	-28.7	-28.9	-30.1	0.017	0.75	18.8	20.9
96018-071	-29.1	-29.2	-30.5	0.038	0.36	14.8	19.7
96018-072	-29.6	-29.3	-30.1	0.019	0.036	18.6	insuff
96018-073	-29.0	-29.3	-29.9	0.021	0.38	4.9	19.8
96018-076	-29.2	-29.2	-29.7	0.048	0.27	19.8	18.8
96018-079	-28.9	-28.9	-30.2	0.22	0.90	13.8	20.8
96018-086	-29.3	-29.1	-30.0	0.29	0.41	13.3	21.2
96018-088	-29.5	-28.9	-29.1	0.10	0.54	1.7	17.8
96018-089	-29.2	-28.5	-27.3	3.9	0.21	-1.7	17.5
96018-092	-29.6	-29.2	-29.2	0.01	0.23	5.8	13.6
96018-093	-30.1	-28.0	-29.7	1.1	0.046	13.0	17.7
96018-094	-29.6	-29.2	-29.8	0.01	0.15	14.3	15.0

Table A6. Extraction and column chromatography data for the Domanik bitumen extracts.

[Note, 96019014-96019017 are oils collected in the vicinity of the Domanik rock samples and, although not discussed in the text, the oil data are included in this table.]

Sample id	Bitumen (ppm-rock)	Sat/Arom ratio	Bitumen on column (mg)	Fractions from column chromatography: Saturates (mg)	Saturates (%)	Aromatics (mg)	Aromatics (%)	NSO (mg)	NSO (%)	Asphaltene (mg)	Asphaltene (%)
96018 001	15421	1.97	49	9.66	24	4.90	12	14.8	37	10.6	27
96018 002	28548	3.13	53	20.6	41	6.59	13	16.4	32	7.27	14
96018 003	27576	1.80	40	6.89	22	3.82	12	13.4	43	7.29	23
96018 004	26962	2.18	47	18.3	38	8.37	17	14.5	30	7.09	15
96018 005	24547	1.67	36	9.20	31	5.52	18	9.88	33	5.32	18
96018 006	23235	2.43	49	17.3	37	7.12	15	14.1	30	7.95	17
96018 007	10105	2.20	52	17.9	37	8.13	17	15.0	31	6.93	14
96018 008	25492	2.04	52	17.3	31	8.46	15	22.6	41	7.01	13
96018 009	21947	2.46	45	17.2	42	6.98	17	12.2	30	4.75	12
96018 010	23777	1.89	49	15.2	33	8.06	17	15.7	34	7.26	16
96018 011	1188	3.16	54	17.0	34	5.38	11	20.5	41	7.61	15
96018 012	7944	2.42	52	16.5	34	6.83	14	15.5	32	9.54	20
96018 016	8577	2.11	40	6.16	20	2.92	10	12.5	41	8.71	29
96018 017	14562	1.25	47	10.5	22	8.44	18	16.7	35	11.9	25
96018 028	5026	1.66	51	13.1	28	7.89	17	15.0	32	10.4	22
96018 029	23279	1.73	52	13.7	29	7.90	16	15.6	33	10.7	22
96018 030	1606	3.84	51	19.6	44	5.11	11	13.4	30	6.47	15
96018 031	5501	3.42	55	16.6	35	4.85	10	20.4	43	6.11	13
96018 034	15784	1.90	51	17.2	37	9.09	19	16.3	35	4.49	10
96018 035	10234	2.21	50	16.2	34	7.34	15	15.6	33	8.60	18
96018 036	14039	1.43	63	9.00	19	6.30	14	21.0	45	10.2	22
96018 037	313	0.58	29	2.04	7.0	3.53	12	8.56	29	15.2	52
96018 044	22244	1.83	44	9.01	25	4.93	14	12.9	36	9.13	25
96018 053	5634	1.12	47	13.2	30	11.8	27	10.3	24	8.51	19
96018 054	13692	1.88	54	15.2	33	8.12	18	14.1	31	8.56	19
96018 055	19833	1.26	46	10.3	25	8.20	20	14.7	36	8.08	20
96018 056	15970	1.51	54	17.2	33	11.4	22	15.3	30	7.84	15
96018 058	15359	1.32	57	18.5	34	14.1	26	15.2	28	6.76	12
96018 059	5476	1.05	49	15.0	32	14.3	30	13.1	28	4.67	10

Table A6. Continued.

Sample id	Bitumen (ppm-rock)	Sat/Arom ratio	Bitumen on column (mg)	Fractions from column chromatography: Saturates (mg)	Saturates (%)	Aromatics (mg)	Aromatics (%)	NSO (mg)	NSO (%)	Asphaltene (mg)	Asphaltene (%)
96018 071	12202	2.51	49	10.6	25	4.20	10	16.4	38	11.6	27
96018 072	2688	2.71	30	10.2	37	3.76	14	8.41	31	4.94	18
96018 073	13227	1.29	51	14.6	30	11.3	23	15.1	31	8.35	17
96018 076	11594	1.65	53	12.9	27	7.82	17	15.8	33	10.7	23
96018 079	19457	1.32	52	17.6	32	13.4	24	12.2	22	12.0	22
96018 086	14698	1.39	51	17.3	34	12.5	24	13.8	27	7.36	14
96018 088	14371	1.55	50	16.2	32	10.4	20	16.7	33	7.66	15
96018 089	1849	1.06	45	11.3	24	10.7	23	16.1	34	9.39	20
96018 092	5451	2.63	51	16.3	34	6.18	13	18.5	39	6.92	14
96018 093	840	1.55	42	12.1	26	7.81	17	14.1	31	12.0	26
96018 094	6197	2.96	46	14.1	36	4.78	12	15.9	41	4.22	11
96019 014		2.18	43	17.8	57	8.14	26	4.08	13	1.29	4.1
96019 015		1.07	51	18.0	41	16.8	38	7.45	17	1.80	4.1
96019 016		2.84	43	18.8	60	6.62	21	3.57	11	2.44	7.8
96019 017		1.70	54	18.7	51	11.0	30	4.67	13	2.16	5.9

Table A7. Biomarker ratios of Domanik bitumen extracts. See parameter key at end of table.

Sample id	depth/strat	TRICY	PENT	STER	C31HSR	C29SR	C29BBAA	T/T+M	TRIOCR	C27STER	C28STER	C29STER
96018 001	0.12	12.80	59.10	28.00	0.58	0.34	0.43	0.66	0.06	0.38	0.17	0.45
96018 002	0.16	33.70	30.90	35.40	0.48	0.36	0.38	0.74	0.11	0.35	0.20	0.46
96018 003	0.20	11.70	57.10	31.20	0.57	0.33	0.43	0.57	0.07	0.25	0.13	0.62
96018 004	0.22	32.30	30.00	37.80	0.45	0.34	0.38	0.75	0.12	0.36	0.19	0.45
96018 005	0.28	11.80	55.70	32.50	0.58	0.37	0.45	0.49	0.06	0.24	0.22	0.54
96018 006	0.32	20.40	47.20	32.40	0.54	0.36	0.41	0.71	0.10	0.34	0.19	0.46
96018 007	0.35	13.60	56.10	30.40	0.59	0.36	0.44	0.56	0.07	0.29	0.20	0.52
96018 008	0.39	14.00	54.30	31.60	0.57	0.37	0.43	0.56	0.06	0.27	0.21	0.52
96018 009	0.42	18.90	52.70	28.40	0.56	0.36	0.42	0.69	0.09	0.32	0.19	0.49
96018 010	0.45	13.80	56.80	29.40	0.58	0.37	0.46	0.59	0.07	0.31	0.20	0.49
96018 011	0.57	15.10	60.20	24.60	0.56	0.35	0.42	0.71	0.05	0.29	0.19	0.51
96018 012	3.90	14.10	57.00	29.00	0.58	0.37	0.40	0.57	0.04	0.32	0.19	0.49
96018 016	9.80	15.10	61.90	23.10	0.55	0.35	0.41	0.70	0.03	0.00	0.28	0.72
96018 017	9.85	20.80	55.80	23.40	0.43	0.27	0.33	0.68	0.08	0.33	0.20	0.47
96018 028	15.25	11.40	59.60	28.90	0.52	0.26	0.36	0.52	0.03	0.29	0.19	0.52
96018 029	15.45	12.40	58.00	29.60	0.50	0.25	0.32	0.58	0.03	0.30	0.18	0.52
96018 030	15.70	9.50	64.10	26.40	0.55	0.25	0.34	0.70	0.02	0.24	0.18	0.58
96018 031	20.67	13.90	55.90	30.20	0.58	0.37	0.40	0.64	0.05	0.27	0.20	0.53
96018 035	20.35	14.00	39.20	46.70	0.44	0.18	0.26	0.39	0.05	0.32	0.17	0.51
96018 036	20.40	5.70	42.90	51.40	0.50	0.18	0.29	0.20	0.01	0.28	0.18	0.54
96018 037	20.73	4.90	49.80	45.30	0.54	0.23	0.28	0.30	0.03	0.32	0.16	0.52
96018 044	19.58	14.90	56.10	29.00	0.57	0.34	0.41	0.60	0.07	0.36	0.18	0.47
96018 053	36.58	17.40	54.90	27.70	0.57	0.43	0.47	0.61	0.14	0.31	0.20	0.48
96018 054	36.80	9.00	69.70	21.30	0.56	0.43	0.45	0.61	0.12	0.29	0.20	0.50
96018 055	37.12	12.60	60.70	26.70	0.56	0.39	0.48	0.56	0.10	0.38	0.11	0.51
96018 056	37.22	10.70	69.20	20.10	0.57	0.41	0.48	0.56	0.11	0.38	0.11	0.51
96018 058	37.54	14.90	55.60	29.60	0.57	0.43	0.46	0.61	0.17	0.33	0.19	0.48
96018 059	38.01	11.40	66.10	22.60	0.55	0.42	0.44	0.60	0.13	0.33	0.20	0.47
96018 063	39.55	15.90	61.80	22.30	0.57	0.48	0.51	0.65	0.02	0.35	0.18	0.47
96018 066	41.00	14.70	57.80	27.50	0.58	0.42	0.48	0.63	0.10	0.36	0.18	0.46
96018 067	41.20	16.80	55.40	27.80	0.57	0.41	0.46	0.61	0.11	0.36	0.18	0.46
96018 070	42.03	15.40	54.10	30.50	0.56	0.42	0.46	0.54	0.12	0.33	0.21	0.47
96018 071	43.42	15.20	58.80	26.00	0.57	0.42	0.47	0.66	0.08	0.26	0.20	0.54

Table A7. Continued.

Sample id	OL/HOP	GAM/HOP	BIS/HOP	DIA/REG	PREG/C27	TRI/HOP	TET/TRI	Ts/Tm	NOR/HOP	NEO/NOR	MOR/HOP
96018 001	0.00	0.11	0.03	0.33	0.07	0.17	0.25	0.51	0.56	0.12	0.12
96018 002	0.01	0.07	0.06	0.47	0.16	0.58	0.30	0.42	0.65	0.10	0.11
96018 003	0.00	0.07	0.02	0.46	0.16	0.16	0.27	0.50	0.61	0.18	0.10
96018 004	0.01	0.05	0.06	0.62	0.17	0.68	0.24	0.37	0.68	0.14	0.16
96018 005	0.01	0.05	0.02	0.41	0.13	0.17	0.23	0.51	0.55	0.10	0.13
96018 006	0.01	0.10	0.02	0.47	0.12	0.29	0.29	0.37	0.64	0.15	0.13
96018 007	0.00	0.06	0.02	0.38	0.15	0.20	0.26	0.52	0.62	0.13	0.09
96018 008	0.00	0.09	0.02	0.44	0.14	0.20	0.23	0.45	0.61	0.12	0.14
96018 009	0.01	0.09	0.03	0.46	0.15	0.25	0.27	0.44	0.61	0.12	0.11
96018 010	0.00	0.02	0.02	0.49	0.13	0.20	0.24	0.52	0.61	0.15	0.13
96018 011	0.00	0.15	0.02	0.30	0.13	0.21	0.26	0.48	0.58	0.13	0.14
96018 012	0.00	0.11	0.03	0.35	0.10	0.19	0.24	0.38	0.56	0.11	0.13
96018 016	0.01	0.06	0.05	0.25	54	0.18	0.25	0.52	0.54	0.14	0.15
96018 017	0.00	0.13	0.06	0.80	0.17	0.17	0.32	0.15	0.53	0.09	0.21
96018 028	0.00	0.26	0.07	0.26	0.11	0.13	0.27	0.45	0.54	0.15	0.16
96018 029	0.00	0.19	0.08	0.25	0.09	0.15	0.30	0.46	0.55	0.13	0.20
96018 030	0.00	0.15	0.06	0.11	0.08	0.11	0.27	0.37	0.52	0.13	0.19
96018 031	0.00	0.09	0.02	0.28	0.17	0.21	0.25	0.43	0.56	0.15	0.12
96018 035	0.00	0.23	0.03	0.16	0.08	0.20	0.25	0.40	0.50	0.11	0.28
96018 036	0.00	0.36	0.03	0.10	0.03	0.11	0.23	0.38	0.47	0.12	0.21
96018 037	0.00	0.41	0.02	1.42	0.07	0.06	0.42	0.23	0.07	6.78	0.24
96018 044	0.00	0.09	0.01	0.25	0.11	0.22	0.22	0.46	0.61	0.13	0.12
96018 053	0.00	0.07	0.01	0.57	0.20	0.26	0.27	0.53	0.64	0.13	0.09
96018 054	0.01	0.09	0.04	0.37	0.17	0.19	0.25	0.65	0.62	0.24	0.15
96018 055	0.00	0.03	0.01	0.31	0.13	0.18	0.24	0.53	0.57	0.12	0.11
96018 056	0.01	0.12	0.04	0.44	0.13	0.19	0.21	0.53	0.57	0.22	0.18
96018 058	0.01	0.04	0.01	0.33	0.20	0.21	0.29	0.58	0.61	0.14	0.08
96018 059	0.01	0.10	0.04	0.41	0.16	0.20	0.21	0.56	0.56	0.17	0.14
96018 063	0.00	0.06	0.02	0.47	0.13	0.21	0.23	0.66	0.59	0.14	0.08
96018 066	0.00	0.06	0.02	0.27	0.14	0.19	0.22	0.60	0.57	0.15	0.09
96018 067	0.00	0.09	0.03	0.36	0.17	0.23	0.27	0.62	0.61	0.16	0.11
96018 070	0.00	0.04	0.02	0.53	0.19	0.23	0.24	0.46	0.64	0.15	0.09
96018 071	0.00	0.06	0.01	0.39	0.22	0.22	0.24	0.65	0.58	0.16	0.09

Table A7. Continued.

Sample id	C32HSR	C35/34	STER/PENT	M/M+T	TRIOCR1	TRIOCR2	TRI/MONO	TRI/STER
96018 001	0.54	0.09	0.47	0.34	0.05	0.07	1.75	0.19
96018 002	0.53	0.06	1.15	0.26	0.12	0.15	2.56	1.51
96018 003	0.55	0.09	0.55	0.43	0.06	0.08	1.28	0.30
96018 004	0.46	0.06	1.26	0.25	0.14	0.17	2.82	1.60
96018 005	0.56	0.07	0.58	0.51	0.05	0.07	0.83	0.32
96018 006	0.52	0.07	0.69	0.29	0.10	0.13	2.19	1.12
96018 007	0.57	0.08	0.54	0.44	0.06	0.08	1.08	0.43
96018 008	0.53	0.08	0.58	0.44	0.06	0.08	1.15	0.46
96018 009	0.57	0.07	0.54	0.31	0.08	0.12	1.88	1.05
96018 010	0.55	0.08	0.52	0.41	0.07	0.09	1.26	0.52
96018 011	0.58	0.07	0.41	0.29	0.05	0.07	2.51	0.35
96018 012	0.56	0.08	0.51	0.43	0.04	0.05	1.11	0.92
96018 016	0.54	0.08	0.37	0.30	0.03	0.03	1.99	0.34
96018 017	0.52	0.09	0.42	0.32	0.09	0.10	1.84	1.47
96018 028	0.50	0.07	0.48	0.48	0.03	0.04	0.89	0.76
96018 029	0.54	0.07	0.51	0.42	0.03	0.04	1.05	1.01
96018 030	0.52	0.09	0.41	0.30	0.02	0.02	2.09	0.12
96018 031	0.58	0.07	0.54	0.36	0.04	0.07	1.68	0.33
96018 035	0.47	0.09	1.19	0.61	0.06	0.06	0.53	0.59
96018 036	0.47	0.12	1.20	0.80	0.01	0.02	0.22	0.16
96018 037	0.54	0.00	0.91	0.70	0.03	0.03	0.37	0.79
96018 044	0.54	0.07	0.52	0.40	0.07	0.09	1.43	0.37
96018 053	0.57	0.06	0.50	0.39	0.15	0.20	1.45	0.80
96018 054	0.59	0.07	0.31	0.39	0.10	0.17	1.32	0.49
96018 055	0.65	0.08	0.44	0.44	0.09	0.14	1.22	0.42
96018 056	0.58	0.06	0.29	0.44	0.11	0.15	1.18	0.50
96018 058	0.58	0.06	0.53	0.39	0.18	0.28	0.89	0.38
96018 059	0.59	0.05	0.34	0.40	0.13	0.18	1.38	0.72
96018 063	0.54	0.09	0.36	0.35	0.02	0.03	1.57	0.40
96018 066	0.56	0.07	0.47	0.37	0.09	0.12	1.60	0.37
96018 067	0.61	0.06	0.50	0.39	0.11	0.15	1.36	0.54
96018 070	0.55	0.07	0.56	0.46	0.13	0.17	1.14	0.69
96018 071	0.60	0.06	0.44	0.34	0.07	0.11	1.73	0.38

Table A7. Continued.

Sample id	depth/strat	TRICY	PENT	STER	C31HSR	C29SR	C29BBAA	T/T+M	TRIOCR	C27STER	C28STER	C29STER
96018 072	43.50	12.80	56.10	31.10	0.58	0.42	0.61	0.62	0.09	0.39	0.18	0.43
96018 073	43.58	23.80	44.30	31.90	0.51	0.43	0.45	0.70	0.25	0.31	0.22	0.47
96018 076	44.79	13.30	55.50	31.20	0.58	0.41	0.46	0.59	0.09	0.26	0.20	0.54
96018 079	45.83	24.20	43.20	32.60	0.55	0.41	0.45	0.68	0.26	0.31	0.20	0.48
96018 086	48.57	16.50	50.40	33.10	0.55	0.42	0.47	0.59	0.15	0.34	0.21	0.46
96018 088	49.63	18.20	47.90	33.90	0.55	0.39	0.43	0.63	0.17	0.26	0.15	0.59
96018 089	50.25	8.80	51.90	39.30	0.32	0.14	0.29	0.11	0.11	0.31	0.16	0.53
96018 092	53.44	14.70	55.30	30.00	0.48	0.32	0.39	0.77	0.13	0.27	0.18	0.54
96018 093	54.76	3.50	37.60	58.90	0.30	0.12	0.19	0.13	0.22	0.26	0.16	0.59
96018 094	55.17	17.90	54.80	27.30	0.54	0.36	0.43	0.72	0.11	0.34	0.19	0.48

Table A7. Continued.

Sample id	OL/HOP	GAM/HOP	BIS/HOP	DIA/REG	PREG/C27	TRI/HOP	TET/TRI	Ts/Tm	NOR/HOP	NEO/NOR	MOR/HOP
96018 072	0.00	0.05	0.01	0.60	0.10	0.17	0.27	0.61	0.56	0.14	0.09
96018 073	0.00	0.09	0.02	1.17	0.32	0.36	0.30	0.44	0.59	0.11	0.12
96018 076	0.00	0.10	0.01	0.35	0.16	0.19	0.26	0.55	0.54	0.18	0.09
96018 079	0.00	0.07	0.03	1.26	0.40	0.37	0.22	0.47	0.65	0.14	0.10
96018 086	0.00	0.06	0.01	0.69	0.12	0.22	0.35	0.51	0.60	0.15	0.11
96018 088	0.00	0.07	0.02	0.83	0.21	0.29	0.27	0.45	0.65	0.11	0.10
96018 089	0.00	0.13	0.27	0.18	0.11	0.04	0.55	0.28	0.37	0.27	0.39
96018 092	0.00	0.12	0.02	0.59	0.26	0.24	0.26	0.40	0.61	0.13	0.12
96018 093	0.00	0.36	0.15	0.06	0.03	0.03	0.53	0.47	0.16	0.14	0.28
96018 094	0.00	0.07	0.02	0.41	0.15	0.26	0.23	0.64	0.60	0.20	0.14

Table A7. Continued.

Sample id	C32HSR	C35/34	STER/PENT	M/M+T	TRIOCR1	TRIOCR2	TRI/MONO	TRI/STER
96018 072	0.57	0.08	0.55	0.38	0.08	0.11	1.47	0.29
96018 073	0.55	0.07	0.72	0.30	0.32	0.50	2.45	1.92
96018 076	0.55	0.07	0.56	0.41	0.08	0.12	1.22	0.40
96018 079	0.55	0.06	0.75	0.32	0.33	0.50	2.43	1.93
96018 086	0.55	0.06	0.66	0.41	0.16	0.22	1.43	0.98
96018 088	0.53	0.06	0.71	0.37	0.18	0.25	1.78	0.86
96018 089	0.28	0.08	0.76	0.89	0.17	0.16	0.14	0.40
96018 092	0.53	0.06	0.54	0.23	0.11	0.17	3.21	0.42
96018 093	0.23	0.10	1.57	0.87	0.23	0.33	0.18	0.16
96018 094	0.56	0.06	0.50	0.28	0.09	0.14	2.40	0.18

Biomarker Parameters Key for Table A7.

Parameter Name:	Description:
TRICY	$$\frac{100 \cdot \sum Tricyclic}{[\ \sum Tricyclic + \sum Pentacyclic + \sum Sterane\ ]}$$
	Where: Σ*Tricyclic* is the sum of all peaks (named and unnamed)in the m/z 191.1800 mass chromatogram from retention time = 0 up to, but not including **C27 18a Ts**; or up to and including **C30 22R Tricyclic** (if **C27 18a Ts** is not present). Σ*Pentacyclic* is the sum of all peaks (named and unnamed)in the m/z 191.1800 mass chromatogram including **C27 18a Ts** and all peaks eluting after **C27 18a Ts** in the m/z 191.1800 mass chromatogram. Σ*Sterane* is the sum of peaks (named and unnamed)in the m/z 217.1956 mass chromatogram including **C27 20S Ba Dia** and all peaks (named and unnamed) eluting thereafter (C_{27} - C_{30} steranes).
PENT	$$\frac{100 \cdot \sum Pentacyclic}{[\sum Tricyclic + \sum Pentacyclic + \sum Sterane]}$$
	Where: Σ*Tricyclic*, Σ*Pentacyclic*, and Σ*Sterane* are defined as above.
STER	$$\frac{100 \cdot \sum Sterane}{[\sum Tricyclic + \sum Pentacyclic + \sum Sterane]}$$
	Where: Σ*Tricyclic*, Σ*Pentacyclic*, and Σ*Sterane* are defined as above.
C31HSR	$$\frac{C_{31}\ 22S\ Hopane}{[C_{31}\ 22S\ Hopane + C_{31}\ 22R\ Hopane]}$$
C29SR	$$\frac{C_{29}\ 20S\ \alpha\alpha\alpha\ Sterane}{[C_{29}\ 20S\ \alpha\alpha\alpha\ Sterane + C_{29}\ 20R\ \alpha\alpha\alpha\ Sterane]}$$
	Where: $\alpha\alpha\alpha$ refers to the $5\alpha(H),14\alpha(H),17\alpha(H)$ steranes.
C29BBAA	$$\frac{C_{29}\ 20R\ \alpha\beta\beta\ Sterane}{[C_{29}\ 20R\ \alpha\beta\beta\ Sterane + C_{29}\ 20R\ \alpha\alpha\alpha\ Sterane]}$$
	Where: $\alpha\alpha\alpha$ refers to the $5\alpha(H),14\alpha(H),17\alpha(H)$ sterane, and

αββ refers to the 5α(H),14β(H),17β(H) sterane.

T/T+M

$$\frac{a}{\left(c \cdot \left\{\left[\frac{b}{a}\right] - 1\right\}\right) + a}$$

Where:
a = **C28 20R Triaromatic Steroid**
b = **C27 20R Triaromatic Steroid**
c = **C29 20R 5a Monoaromatic Steroid**
d = **C28 20R5a+C29 20R5B Monoaromatic Steroi**
or, if the peaks are resolved,
d = **C28 20R 5a Monoaromatic Steroid** +
C29 20R 5B Monoaromatic Steroid

TRIOCR

$$\frac{(C_{20}\ \text{Triaromatic Steroid} + C_{21}\ \text{Triaromatic Steroid})}{\sum \text{Triaromatic Steroids}}$$

Where:
ΣTriaromatic Steroids is the sum of <u>all</u> peaks (named and unnamed)in the m/z 231.1174 mass chromatogram.

C27STER

$$\frac{C_{27}\ 20R\ \alpha\alpha\alpha\ \text{Sterane}}{(C_{27}\ 20R\ \alpha\alpha\alpha\ \text{Sterane} + C_{28}\ 20R\ \alpha\alpha\alpha\ \text{Sterane} + C_{29}\ 20R\ \alpha\alpha\alpha\ \text{Sterane})}$$

C28STER

$$\frac{C_{28}\ 20R\ \alpha\alpha\alpha\ \text{Sterane}}{(C_{27}\ 20R\ \alpha\alpha\alpha\ \text{Sterane} + C_{28}\ 20R\ \alpha\alpha\alpha\ \text{Sterane} + C_{29}\ 20R\ \alpha\alpha\alpha\ \text{Sterane})}$$

C29STER

$$\frac{C_{29}\ 20R\ \alpha\alpha\alpha\ \text{Sterane}}{(C_{27}\ 20R\ \alpha\alpha\alpha\ \text{Sterane} + C_{28}\ 20R\ \alpha\alpha\alpha\ \text{Sterane} + C_{29}\ 20R\ \alpha\alpha\alpha\ \text{Sterane})}$$

OL/HOP

$$\frac{C_{30}\ \text{Oleanane}}{C_{30}\ \text{Hopane}}$$

GAM/HOP

$$\frac{C_{30}\ \text{Gammacerane}}{C_{30}\ \text{Hopane}}$$

BIS/HOP

$$\frac{\text{Bisnorhopane}}{C_{30}\ \text{Hopane}}$$

DIA/REG

$$\frac{C_{27}\ 20S\ \beta\alpha\ \text{Diasterane}}{C_{29}\ 20R\ \alpha\alpha\alpha\ \text{Sterane}}$$

Where:
βα Diasterane refers to the 13β(H),17α(H) Diasterane
(sometimes called "rearranged" sterane)

PREG/C27 $$\frac{\text{Pregnane}}{C_{27}\ 20R\ \alpha\alpha\alpha\ \text{Sterane}}$$

TRI/HOP $$\frac{C_{23}\ \text{Tricyclic}}{C_{30}\ \text{Hopane}}$$

TET/TRI $$\frac{C_{24}{*}\ \text{Tetracyclic}}{C_{23}\ \text{Tricyclic}}$$

Ts/Tm $$\frac{C_{27}\ 18\alpha\ \text{Trisnorhopane (Ts)}}{C_{27}\ 17\alpha\ \text{Trisnorhopane (Tm)}}$$

NOR/HOP $$\frac{C_{29}\ \text{Norhopane}}{C_{30}\ \text{Hopane}}$$

NEO/NOR $$\frac{C29\ 18\alpha\ \text{Neonorhopane}}{C_{29}\ \text{Norhopane}}$$

MOR/HOP $$\frac{(C_{29}\ 17\beta\ 21\alpha\ \text{Normoretane} + C_{30}\ 17\beta\ 21\alpha\ \text{Moretane})}{(C_{29}\ \text{Norhopane} + C_{30}\ \text{Hopane})}$$

C32HSR $$\frac{C_{32}\ 22S\ \text{Hopane}}{[C_{32}\ 22S\ \text{Hopane} + C_{32}\ 22R\ \text{Hopane}]}$$

C35/C34 $$\frac{(C_{35}\ 22S\ \text{Hopane} + C_{35}\ 22R\ \text{Hopane})}{\sum_{n=31}^{n=34}(C_n\ 22S\ \text{Hopane} + C_n\ 22R\ \text{Hopane})}$$

STER/PENT $$\frac{\sum Sterane}{\sum Pentacyclic}$$

Where:
Σ*Sterane* and Σ*Pentacyclic* are defined as above.

M/M+T 1-(T/T+M)

TRIOCR1 $$\frac{C_{20}\ \text{Triaromatic}}{(C_{20}\ \text{Triaromatic} + C_{28}\ 20S\ \text{Triaromatic} + C_{28}\ 20R\ \text{Triaromatic})}$$

TRIOCR2 $$\frac{(C_{20}\ \text{Triaromatic} + C_{21}\ \text{Triaromatic})}{\sum \text{Identified } C_{26} - C_{28}\ \text{Triaromatics}}$$

TRI/MONO

$$\frac{\sum Triaromatic}{\sum Monoaromatic}$$

Where:
Σ*Triaromatic* is the sum of peaks (named and unnamed)in the m/z 231.1174 mass chromatogram and Σ*Monoaromatic* is the sum of peaks (named and unnamed)in the m/z 253.1956 mass chromatogram.

TRI/STER

$$\frac{\sum Triaromatic}{\sum Sterane}$$

Where:
Σ*Triaromatic* and Σ*Sterane* are defined as above.

Table A8. Saturated hydrocarbon gas chromatography data for Domanik bitumen extracts. See parameter key at end of table.

Sample id	Comments	Pr/Ph area	Pr/Ph height	Pr/17 area	Pr/17 height	Ph/18 area	Ph/18 height	CPI 1 area	CPI 1 height	CPI 2 area	CPI 2 height	CPI 3 area	CPI 3 height	CPI 4 area
96018 001	mod. biodegraded	1.07	1.34	2.48	2.85	4.58	3.31					1.62	1.49	7.61
96018 002	-0-	1.61	1.66	0.77	0.62	0.62	0.44					0.99	0.92	1.02
96018 003	mod. biodegraded	1.54	1.59	1.94	1.95	1.99	1.57					1.34	1.29	1.9
96018 004	-0-	1.59	1.7	0.76	0.6	0.62	0.43	1.01	1.01			0.94	0.9	0.99
96018 005	mod. biodegraded	1.15	1.33	3.37	4.27	23.64	17.25					0.75	0.81	1.18
96018 006	-0-	1.5	1.62	0.97	0.76	0.76	0.54	1.02	1.01	1.02	1.02	1	0.95	1.01
96018 007	-0-	1.48	1.61	1.04	0.94	1.04	0.71					0.52	0.84	0.99
96018 008	-0-	1.51	1.59	1.22	1.12	1.18	0.84					0.51	0.69	1.01
96018 009	-0-	1.63	1.62	0.98	0.77	0.77	0.56	1.01	1.01	1.02	1.02	1.02	1.01	0.98
96018 010	-0-	1.36	1.49	1.29	1.13	1.18	0.86	1.15	1.05	1.15	1.03	0.96	0.97	1.04
96018 011	-0-	1.31	1.41	1.24	0.99	1.07	0.79	1	0.97	1.01	0.98	1.11	1	0.97
96018 012	-0-	1.31	1.41	1.67	1.38	1.5	1.11	0.93	0.97	0.93	0.98	0.97	1.02	0.96
96018 016	mod. biodegraded	0.89	1.16	5.83	5.23	8.97	6.64	1.05	1.27	0.99	1.14	1.39	1.77	2.63
96018 017	-0-	1.36	1.53	1.28	1.11	1.14	0.87	0.97	0.99			0.81	1.04	0.99
96018 028	-0-	1.42	1.43	1.25	1.05	1.13	0.83	0.97	0.97	0.96	0.94	0.96	0.93	0.95
96018 029	-0-	1.24	1.37	1.32	1.07	1.12	0.8	1.01	0.99	1.03	1	0.84	0.84	0.97
96018 030	minor biodegraded	0.82	0.87	3.43	3.67	3.43	2.72	1.07	0.97	1.09	0.99	1.16	0.98	0.99
96018 031	-0-	1.19	1.31	2.22	2.09	1.89	1.63	1.09	1.01	1.1	1.03	1.29	1.07	0.98
96018 034	-0-	1.33	1.44	1.94	1.64	1.59	1.3	1.01	0.99	1.03	1	0.97	1.03	0.91
96018 035	-0-	1.5	1.61	1.19	0.94	0.95	0.68	0.96	1	0.96	1.01	0.96	1	0.9
96018 036	-0-	1.3	1.39	2.93	2.71	3.31	2.18	0.57	0.56	0.52	0.53	0.35	0.42	0.69
96018 037	-0-	1.02	1.07	3.64	2.85	3.68	2.59	1.07	1.05	1.06	1.02	1.36	1.33	0.98
96018 044	severe biodegradation													
96018 053	mod. biodegraded	0.96	1.38	2.4	3.42	12.57	4.93					1.05	1.02	1.53
96018 054	severe biodegradation													
96018 055	severe biodegradation													
96018 056	severe biodegradation													
96018 058	severe biodegradation													

Table A8. Continued.

Sample id	CPI 4 height	OEP 1 area	OEP 1 height	OEP 2 area	OEP 2 height	OEP 3 area	OEP 3 height
96018 001	4.21	4.11	2.18	1.25	1.17		
96018 002	0.99	0.94	0.92	1.03	1		
96018 003	1.63	1.74	1.51	1.06	1.04		
96018 004	1	0.91	0.93	0.97	0.96	1.2	1.2
96018 005	1.23	0.79	0.84	0.59	0.65		
96018 006	1	0.9	0.93	0.99	0.98	0.98	0.98
96018 007	1.08	1.03	1.13	0.5	0.78		
96018 008	1.04	0.98	1.02	0.52	0.71		
96018 009	1	0.9	0.94	1.01	1.02	1.11	1.11
96018 010	1.01	0.97	0.96	1.03	0.99	1.64	1.64
96018 011	0.96	0.94	0.94	1.08	1	1.05	1.05
96018 012	0.95	0.92	0.94	0.94	1.01	0.81	0.81
96018 016	2.35	2.62	2.01	1.15	1.48	0.6	0.6
96018 017	0.98	0.9	0.93	0.81	1.04	0.84	0.84
96018 028	0.98	0.89	0.95	0.92	0.91	1.02	1.02
96018 029	1	0.9	0.98	0.87	0.88	1.3	1.3
96018 030	0.95	0.95	0.93	1.12	0.97	1.25	1.25
96018 031	0.95	0.97	0.95	1.24	1.05	1.34	1.34
96018 034	0.94	0.83	0.88	0.99	1.04	1.59	1.59
96018 035	0.97	0.84	0.92	0.99	1.04	1.55	1.55
96018 036	0.58	0.49	0.42	0.34	0.39	0.57	0.57
96018 037	0.97	0.85	0.84	1.26	1.24	1.42	1.42
96018 044							
96018 053	1.33	0.89	0.69	0.84	0.82		
96018 054							
96018 055							
96018 056							
96018 058							

Table A8. Continued.

Sample id	Comments	Pr/Ph area	Pr/Ph height	Pr/17 area	Pr/17 height	Ph/18 area	Ph/18 height	CPI 1 area	CPI 1 height	CPI 2 area	CPI 2 height	CPI 3 area	CPI 3 height	CPI 4 area
96018 066	severe biodegradation													
96018 067	severe biodegradation													
96018 070	severe biodegradation													
96018 071	severe biodegradation													
96018 072	mod. biodegraded	1.23	1.31	6.79	8.68	9.63	7.94					0.88	0.89	0.85
96018 073	severe biodegradation													
96018 076	severe biodegradation													
96018 079	mod. biodegraded	1.6	1.57	3.94	6.05	5.64	4.45	0.99	0.95	0.93	0.92	1.03	0.97	1.02
96018 086	mod. biodegraded	1.67	1.49	53.44	38.89	4.13	3.01					0.91	0.98	1.21
96018 088	-0-	1.58	1.7	2.19	1.92	1.7	1.25	1.1	1.01	1.14	1.03	1.26	0.97	1.06
96018 089	minor biodegraded	1.27	1.31	3.4	2.68	3.06	2.38	0.99	0.95	0.98	0.93	0.97	0.9	0.99
96018 092	-0-	1.51	1.61	1.01	0.8	0.82	0.61	1.04	1.03	1.06	1.05	1.33	1.22	0.96
96018 093	-0-	1	1.06	1.39	1.15	2.16	1.67	0.9	0.96	0.91	0.94	0.89	0.67	0.97
96018 094	minor biodegraded	1.22	1.27	5.36	5.44	3.09	2.58	0.97	0.99	0.96	1	0.98	1	1.01

Table A8. Continued.

Sample id	CPI 4 height	OEP 1 area	OEP 1 height	OEP 2 area	OEP 2 height	OEP 3 area	OEP 3 height
96018 066							
96018 067							
96018 070							
96018 071							
96018 072	0.86	1.02	0.9	0.72	0.75		
96018 073							
96018 076							
96018 079	0.99	0.93	0.97	0.96	0.93	0.85	0.85
96018 086	1.15	0.43	0.45	0.69	0.75		
96018 088	1	1.03	0.97	1.21	0.98	1.24	1.24
96018 089	0.96	0.87	0.87	0.92	0.88	0.96	0.96
96018 092	0.96	0.94	0.95	1.29	1.21	1.49	1.49
96018 093	0.97	0.95	0.86	0.84	0.72	0.78	0.78
96018 094	0.97	1	0.97	0.94	0.99	0.88	0.88

Notes:

HMW = high molecular weight (greater than n-C22)
Pr/Ph = pristane/phytane
Pr/17 = pristane/n-C17
Ph/18 = phytane/n-C18
CPI = Carbon Preferential Index
OEP = Odd Even Predominance

$$OEP = \left(\frac{C_i + 6C_{i+2} + C_{i+4}}{4C_{i+1} + 4C_{i+3}}\right)^{(-1)^{i+1}}$$

Scalan and Smith (1970)

OEP 1 = centered on n-C27 (i = 25)
OEP 2 = centered on n-C29 (i = 27)
OEP 3 = centered on n-C31 (i = 29)

$$CPI\ 1 = \frac{1}{2} \times \left(\frac{C_{23} + C_{25} + C_{27} + C_{29} + C_{31}}{C_{24} + C_{26} + C_{28} + C_{30} + C_{32}} + \frac{C_{25} + C_{27} + C_{29} + C_{31} + C_{33}}{C_{24} + C_{26} + C_{28} + C_{30} + C_{32}}\right)$$

Hunt (1979)

$$CPI\ 2 = \frac{1}{2} \times \left(\frac{C_{25} + C_{27} + C_{29} + C_{31} + C_{33}}{C_{24} + C_{26} + C_{28} + C_{30} + C_{32}} + \frac{C_{25} + C_{27} + C_{29} + C_{31} + C_{33}}{C_{26} + C_{28} + C_{30} + C_{32} + C_{34}}\right)$$

Bray and Evans (1961)

$$CPI\ 3 = 2 \times \left(\frac{C_{29}}{C_{28} + C_{30}}\right)$$

Philippi (1965)

$$CPI\ 4 = \left(\frac{(C_{23} + C_{25} + C_{27}) + (C_{25} + C_{27} + C_{29})}{2 \times (C_{24} + C_{26} + C_{28})}\right)$$

based on Marzi and others (1993)