PETROGRAPHIC AND GEOCHEMICAL STUDY OF COALS FROM THE SANTA TEREZINHA COALFIELD, RIO GRANDE DO SUL, BRAZIL

ARAÚJO, C. V.[1]; CORRÊA DA SILVA, Z. C.[2] and RODRIGUES, R.[1]

[1]Petrobrás/Cenpes/Divex, Cidade Universitária, Quadra 7, Ilha do Fundão,
Rio de Janeiro, RJ, 21949-900, Brazil
[2]Universidade Federal do Rio Grande do Sul, Institute of Geosciences

ABSTRACT—Several coal seams from the Santa Terezinha Coalfield, northeast of the State of Rio Grande do Sul, Southern Brazil, were studied on the basis of petrographic and geochemical techniques.

The coals are rich in mineral matter . The vitrinite content reaches 72% and inertinite 58%. The content of liptinite is low (up to 14%).

Among the microlithotypes, carbominerite and vitrite are predominant. Vitrinite reflectance, moisture (ash free basis) and volatile matter (dry ash free basis) of hand picked vitrain indicated the coals to reach a rank of High Volatile Bituminous A/B. Some coal layers were thermally affected by igneous intrusive bodies.

The microlithotype association indicated that open moor conditions (limnic facies) prevailed during the formation of the coal seams. Pristane/phytane ratios are always higher than 2, reaching up to 7.4.

The terpane analysis showed higher relative abundance of tetracyclic over tricyclic compounds, predominance of C_{19} and C_{20} tricyclic terpanes, high relative abundance of trisnorhopane (Tm), norhopane and βα hopanes. The investigation of steranes showed a predominance of C_{29} compounds as well as a low sterane/hopane ratio (<O. 1).

Some remarkable characteristics in maceral composition and stable carbon isotopes allowed the subdivision of the sequence in four groups of samples (A, B, C and C*).

RESUMO —Foram realizadas análises de geoquímica e petrografia orgânicas de várias camadas e leitos de carvão de duas sondagens realizadas na Jazida Carbonífera de Santa Terezinha, na região nordeste do Estado do Rio Grande do Sul.

Os carvões estudados são ricos em matéria mineral. Dentre os macerais predominam os do grupo da vitrinita que chegam a atingir 72%, seguidos pela inertinita com 58%. 0 conteúdo em liptinita é baixo, não ultrapassando 14%.

Os microlitotipos predominantes são carbominerita e vitrita.

A determinação do grau de carbonificação ("rank") foi feita através da reflectância da vitrinita, umidade (isenta de cinzas) e matéria volátil (seca isenta de cinzas) de amostras de vitrênio puro e os resultados obtidos permitiram classificar os carvões como correspondentes ao estágio Betuminoso de Alto Volátil A/B, de acordo com as normas ASTM. Os níveis carbonosos afetados por intrusões ígneas apresentam um "rank"mais elevado.

As associações de microlitotipos indicaram que condições límnicas de águas abertas prevaleceram durante a formação das camadas de carvão.

As razões Pristano/Fitano são sempre maiores que 2, chegando a alcançar 7,4. As análises de terpanos mostraram uma abundância relativa de compostos tetracíclicos sobre os tricíclicos, predominância dos terpanos tricíclicos C_{19} e C_{20}, bem como altos teores de trisnorhopano (Tm), norhopano e βα hopanos. A análise de esteranos mostrou a predominância de compostos em C_{29} bem como uma baixa razão esteranos/hopanos(<0,1).

Os carvões estudados foram divididos em quatro grupos (A, B, C e C*) de composição macerálica diferente e com valores distintos de isótopos estáveis de Carbono.

INTRODUCTION

Santa Terezinha Coalfield is located in the northeastern region of the State of Rio Grande do Sul (Fig. 1). Several boreholes were drilled in the area by the Companhia de Pesquisas de Recursos Minerais (CPRM). The samples used for this study were collected from the cores of two of these boreholes (2TG-227-RS and 2TG-230-RS).

According to Fabricio et al. (1980) seven coal seams or layers occur named from top to bottom Santa Terezinha 1 through Santa Terezinha 7 (ST1-ST7). The most important seam from the economical point of view is Santa Terezinha 4 due to its thickness and areal distribution.

The Santa Terezinha coal measures are part of the Rio Bonito Formation, Guatá Group, Tubarão Supergroup (Artinskian/Kungurian Age) of the Paraná Basin (Schneider et al., 1974).

The purpose of this study is to characterize the coal seams in terms of organic petrography and geochemistry in order to approach the rank and organic facies.

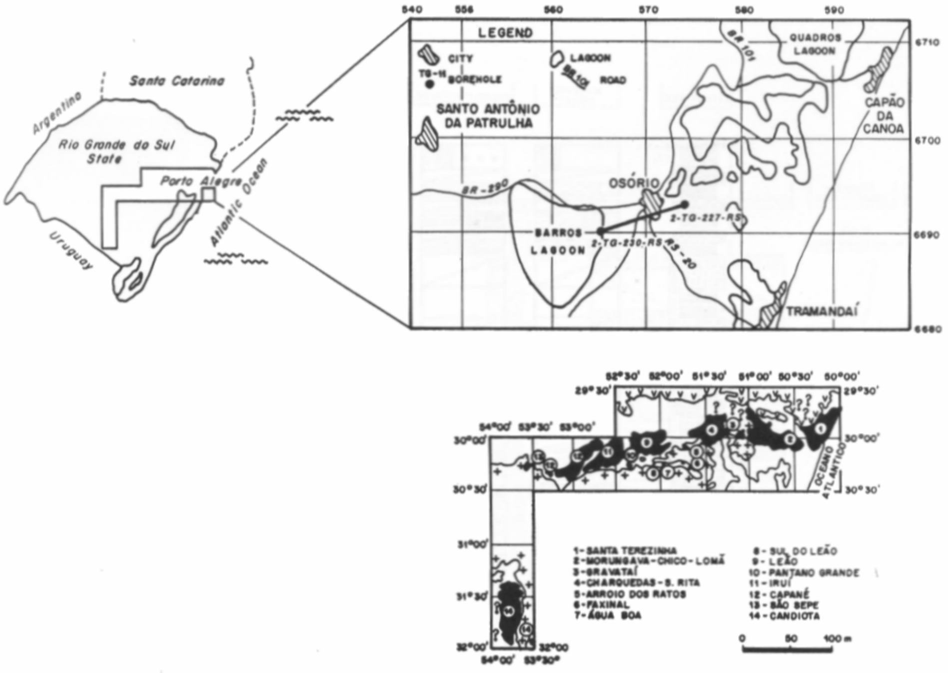


Figure 1. *Coalfields of the state of Rio Grande do Sul (DNPM-CPRM, 1986) and the location map of the Santa Terezinha area with 2TG-227-RS and 2TG-230-RS boreholes.*

ANALYTICAL METHODS

The coal measures were described according to Corrêa da Silva & Marques Toigo (1975) and Schopf (1960). Samples were collected following the macroscopic description of lithotypes according to Hacquebard & Donaldson (1969). Each sample was split to make polished sections, proximate and geochemical analyses.

For microscopic studies the samples were crushed to a size between 1.00 and 0.81 mm, embedded in resin (Araldite), ground and polished. Maceral and microlithotypes composition were determined by combined analysis using a Kotter's 20-point graticule (Stach et al., 1982). About 6,000 points per sample were counted in reflected white light on a Orthoplan-pol Leitz Photomicroscope with objectives of 50x0.85 oil. Vitrinite reflectance (Rr%) was measured on telocollinites in oil immersion at 546nm, and mean values for each sample were calculated. Fluorescence of liptinite macerals was observed on a Zeiss Photomicroscope with a HBO mercury lamp and Plan-Neofluar 25./8 water objective.

Bitumen was extracted in a Soxhlet Apparatus by refluxing with dicloromethane. The organic extracts were fractionated via column-liquid chromatography. The GC analyses of alkanes were carried out using a high resolution Varian 3700 chromatograph equipped with a split injector and fitted with a 25mx0.33mm SE-54 column. Hydrogen was employed as carrier gas with a temperature program of 40-280°C at 8°C/min. The GC-MS analyses were performed using a Varian 3700 chromatograph, a Varian 112-5 mass spectrometer coupled with a Varian 55- 100-MS data acquisition system. The GC-MS-MS analyses were performed on a TSQ-70 tandem mass spectrometer. Carbon isotope analyses were undertaken using a vacuum combustion line linked to a Varian MAT230 instrument. The data are presented in delta notation ($\delta^{13}C$‰) relative to Pee Dee Belemnite (PDB).

RESULTS

Petrography

The macroscopic description of the coal shows, in terms of lithotypes, a slight predominance of fine banded coal and a significant occurrence of dull coal (Figs. 2 and 3).

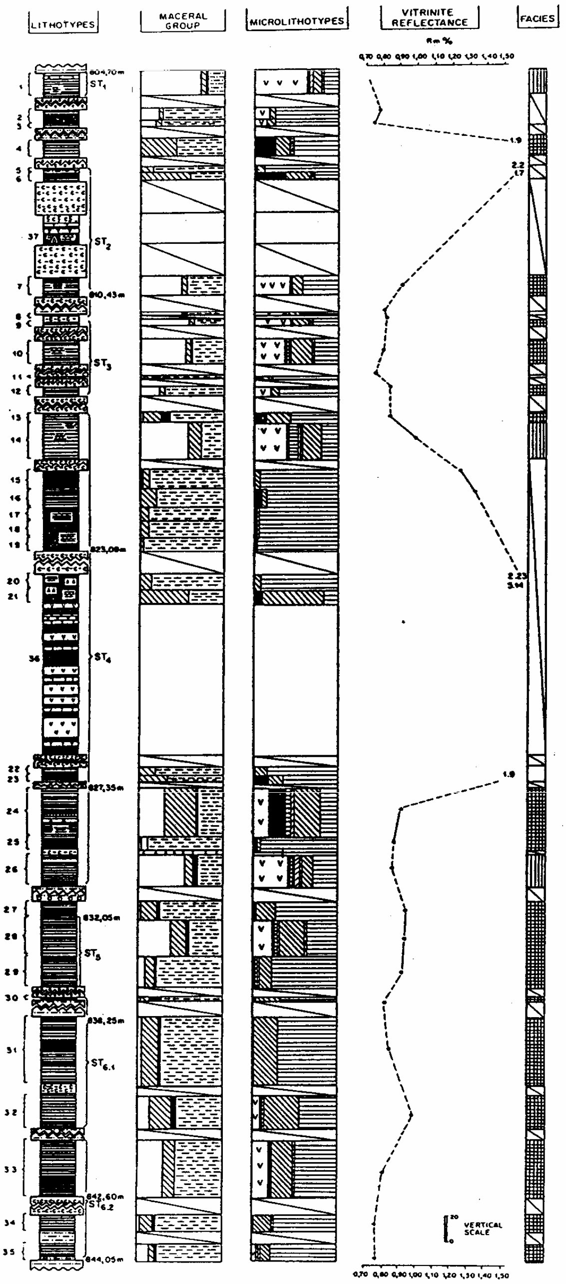


Figure 2. *Section of lithotypes, maceral groups, microlithotypes, range of mean vitrinite reflectance (Rr%) and facies of 2TG-227-RS borehole. ST_1 = seam identification.*

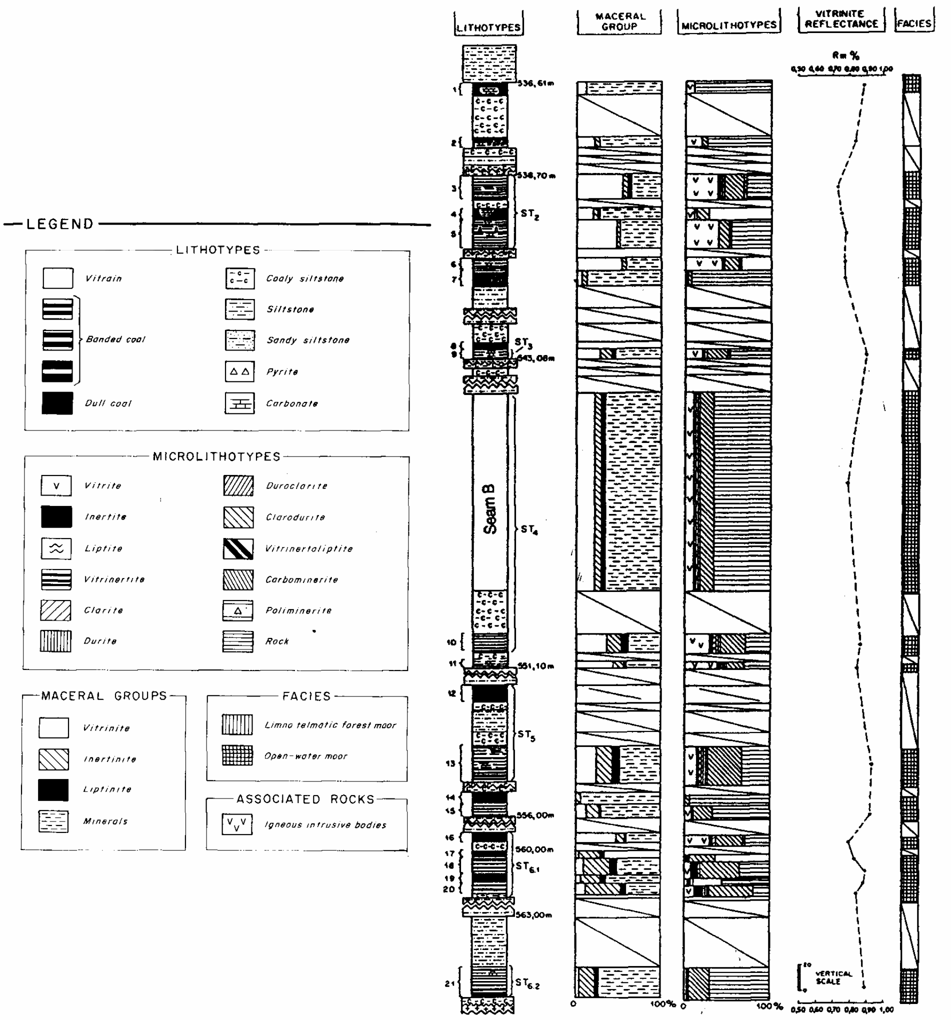


Figure 3. *Section of lithotypes, maceral groups, microlithotypes, range of mean vitrinite reflectance (Rr%) and facies of 2TG-230-RS borehole. ST_i = seam identification.*

Maceral Analysis

Microscopic analysis (Araujo, 1990) reveals abundant mineral matter (Figs. 2 and 3; Tables 1 and 2). Clays are the dominant minerals and carbonate and pyrite also occur. Only few intervals in both boreholes present mineral matter contents lower than 50%.

In several intervals the content of vitrinite is high, mostly toward the top of the section. In this group the occurrence of telocollinite (mostly with resin impregnations), desmocollinite, gelocollinite, vitrodetrinite and telinite is significant. The occurrence of macerals of the inertinite group is also expressive, specially fusinite and inertodetrinite.

In general, the liptinite group is slightly more abundant in coals from the borehole 2TG-230-RS than in these from 2TG-227-RS. The contents of liptinite tend to be higher below seam ST4 and the most frequent macerals are liptodetrinite, microsporinite, macrosporinite, resinite, cutinite, and alginite.

Both ST2 and ST4 seams, in borehole 2TG-227-RS, are affected by igneous intrusions that caused thermal alteration of the organic matter.

Microscopic observations under UV-light revealed that vitrinite, particularly gelocollinite, exhibits a dark orange fluorescence.

Microlithotype Analysis

The study of microlithotypes showed the predominance of carbominerite, rock[1] and vitrite. Carbargilite is more abundant than carbopyrite and carbankerite. Rock is basically composed of clay. Clay is frequently associated with liptodetrinite, filamentous alginite and tenuisporinite.

Vitrite is mostly telocollinite and gelocollinite. Inertite is composed of fusinite, semifusinite and inertodetrinite, followed by sclerotinite and

Sample number	Seam	Maceral Group				Microlithotypes												
		V	L	I	M	Vi	Li	In	Cl	Du	Vt	Dc	Cd	Vtl	Cm	P	R	Isol.
01	ST_1	72	2	6	20	63,4	-	2,3	4,6	-	-	0,3	-	-	11,1	1,3	17,0	-
02		2	-	5	73	18,4	-	0,8	-	-	-	-	-	-	5,2	0,6	75,0	-
03		18	1	6	75	12,9	-	0,5	-	-	-	0,3	-	-	9,8	0,5	76,0	-
04	Coal bed I	-	-	42	58	-	-	25,0	-	-	-	-	-	-	18,3	3,4	53,3	-
05		-	-	15	85	-	-	2,0	-	-	-	-	-	-	7,7	-	90,3	-
06	ST_2	-	-	58	42	-	-	34,4	-	-	-	-	-	-	30,6	4,1	30,9	-
07		49	-	5	46	41,7	-	1,3	1,0	-	0,3	-	-	-	11,4	0,3	44,0	-
08		49	2	3	46	33,8	-	1,1	1,3	-	1,1	-	-	-	17,9	1,6	33,2	-
09		57	1	5	37	42,2	0,3	0,3	2,3	-	-	-	-	-	20,8	3,9	29,9	-
10	ST_3	53	2	5	40	36,1	0,5	1,2	2,6	-	1,0	0,3	-	-	25,5	1,0	31,7	-
11		5	1	8	76	25,0	1,8	1,5	0,3	-	0,3	-	-	-	15,4	0,8	78,4	-
12		22	5	5	73	18,2	0,8	-	-	-	-	-	-	-	10,5	-	70,2	-
13		3	10	21	66	0,9	1,2	7,8	-	1,2	0,3	-	0,3	-	29,4	0,6	58,3	-
14		55	1	15	29	38,8	-	2,5	1,7	-	11,3	2,2	0,3	-	22,3	-	20,9	-
15		1	-	9	90	0,8	-	0,8	-	-	-	-	-	-	6,9	-	91,5	-
16		-	-	17	83	0,3	-	8,9	-	-	-	-	-	-	6,4	0,3	84,1	-
17		-	-	8	92	-	-	2,7	-	-	0,2	-	-	-	2,4	-	94,7	-
18		-	-	8	92	-	-	1,6	-	-	-	-	-	-	1,9	-	96,5	-
19	ST_4	1	-	2	97	-	-	0,3	-	-	-	-	-	-	1,4	-	98,3	-
20		-	-	12	8	-	-	0,2	-	-	-	-	-	-	6,5	-	93,3	-
21		-	-	55	45	7,0	-	-	-	-	-	-	-	-	74,2	0,8	18,0	-
22		-	-	18	82	-	-	1,6	-	-	-	-	-	-	14,2	-	84,1	0,1
23		-	-	34	66	-	-	18,5	-	-	-	-	-	-	17,7	0,3	63,5	-
24		29	3	38	30	19,4	0,3	18,6	0,6	0,3	5,8	1,7	0,3	0,3	32,6	0,3	19,9	-
25		2	1	8	89	1,4	-	1,7	0,3	-	-	-	-	-	4,2	-	92,4	-
26		54	6	9	31	46,4	0,6	2,3	1,1	1,4	3,7	5,1	0,6	1,7	15,1	0,9	25,1	-
27		3	4	19	74	1,7	0,3	2,7	-	0,6	-	-	-	-	23,1	0,3	71,3	-
28	ST_5	37	4	18	41	24,4	0,6	2,0	1,7	0,8	3,5	2,3	0,3	-	29,9	2,6	31,9	-
29		8	3	12	77	2,6	0,3	1,4	0,3	0,8	1,1	1,1	-	-	15,0	0,5	76,8	-
30		2	14	13	71	-	0,3	1,2	-	1,2	-	0,3	-	0,3	20,9	0,3	66,5	-
31	$ST_{6.1}$	3	5	20	72	0,8	0,3	1,6	-	0,8	-	0,3	-	-	28,3	0,3	67,6	-
32		15	6	26	53	9,3	0,9	1,2	0,3	0,3	2,2	0,9	-	-	42,0	0,9	41,9	-
33		29		14	57	20,9	-	3,5	-	-	0,3	0,3	-	-	26,2	2,2	46,4	0,1
34	$ST_{6.2}$	2	3	17	78	0,2	0,3	1,8	-	-	0,3	-	-	-	22,7	1,6	72,9	0,2
35		13	3	6	78	7,0	-	0,3	1,7	0,5	0,8	1,7	0,5	0,3	10,8	0,8	75,6	-

Table 1. *Results of combined analysis of maceral groups and microlithotypes of coal samples from borehole 2TG-227-RS, Santa Terezinha Coal Field, Rio Grande do Sul Brazil.*

V - vitrinite L - liptinite I - inertinite M - minerals;
Vi - vitrite Li - liptite In - inertite Cl - clarite Du - durite Vt - vitrinertite
Dc - duroclarite Cd - clarodurite Vtl - vitrinertoliptite Cm - carbominerite
P - poliminerite R - Rock Isol - isolated maceral (less than 10 intersections fall inside the coal particle)

---

[1] **Rock,** not common in northern hemisphere coals, is defined as having more than 10% of pyrite or more than 60% of clay or carbonate (Stach et al. 1982).

Sample number	Seam	Maceral Group				Microlithotypes											
		V	L	I	M	Vi	Li	In	Cl	Du	Vt	Dc	Cd	Vtl	Cm	P	R
01		11	-	-	89	9,7	-	-	0,6	-	-	-	-	-	0,6	-	89
02		20	-	7	73	-	17,6	-	0,8	0,3	-	-	-	-	6,5	-	74,3
03	ST_2	54	4	5	37	37,8	1,2	0,6	2,9	-	-	1,2	-	-	23,6	2,9	29,8
04		18	2	6	74	10,7	-	0,6	1,4	-	0,3	-	-	-	14,2	0,5	72,2
05		47	-	4	49	37,3	-	0,5	0,5	-	-	0,3	-	-	12,8	2,3	36,2
06	Coal bed 1	52	1	6	41	42,7	-	1,2	0,3	-	-	-	-	-	18,6	2,1	25,1
07		4	-	5	91	1,5	-	0,3	-	-	-	-	-	-	3,9	0,6	93,6
09	ST_3	27	4	13	56	19,0	0,6	2,0	1,7	0,3	0,3	0,6	-	-	24,0	2,5	49,0
10	ST_4	35	7	18	40	25,3	0,6	4,4	1,1	0,6	3,6	2,7	0,8	0,8	29,1	0,3	30,6
11		43	12	14	41	35,3	-	3,8	1,9	-	1,4	1,9	0,8	-	20,8	0,5	33,4
12	ST_5	25	7	20	48	14,2	0,3	2,6	1,9	1,1	1,9	1,0	-	-	40,3	0,8	35,9
14		-	-	5	95	-	-	-	-	-	-	-	-	-	4,3	-	95,7
15		13	2	15	70	6,7	-	1,7	0,6	-	0,3	0,6	-	-	22,5	-	67,7
16	$ST_{6.1}$	48	2	10	40	27,7	-	2,6	4,0	-	0,6	0,3	-	-	32,6	1,1	31,2
17		4	4	26	66	0,3	-	3,6	0,6	-	0,6	0,6	-	-	30,4	0,6	63,2
18		10	8	31	51	5,9	-	7,2	-	1,1	0,9	1,4	0,3	0,5	45,1	0,5	37,0
19		6	6	25	63	2,1	-	3,4	-	0,3	1,6	0,8	0,3	-	33,0	-	58,5
20		11	7	42	40	9,8	-	9,9	1,7	1,4	0,9	1,3	0,8	0,3	52,1	-	21,8
21	$ST_{6.2}$	2	3	22	72	1,4	0,5	1,9	-	-	0,5	0,3	-	-	24,6	0,3	70,5

Table 2. *Results of combined analysis of maceral groups and microlithotypes of coal samples from borehole 2TG-230-RS, Santa Terezinha Coal Field, Rio Grande do Sul, Brazil.*

V - vitrinite L - liptinite I - inertinite M - minerals;
Vi - vitrite Li - liptite In - inertite Cl - clarite Du - durite Vt - vitrinertite
Dc - duroclarite Cd - clarodurite Vtl - vitrinertoliptite Cm - carbominerite P - poliminerite R - Rock

Seam	Sample number	Rr%	Rr% range	number of measurements	standard deviation
ST_1	1	0,71	(0,64-0,83)	188	0,04
	2	0,78	(0,72-0,90)	171	0,03
	3	0,75	(0,70-0,80)	87	0,03
	4	1,91	(1,43-2,17)	43	0,19
ST_2	5	2,16	(1,90-2,71)	45	0,23
	6	1,72	(1,51-2,00)	62	0,11
	7	0,91	(0,81-1,06)	135	0,06
	8	0,80	(0,75-0,87)	94	0,03
ST_3	9	0,81	(0,79-0,87)	143	0,03
	10	0,80	(0,70-0,84)	124	0,03
	11	0,76	(0,76-0,85)	42	0,04
	12	0,85	(0,80-0,93)	82	0,03
ST_4	13	0,84	(0,74-0,97)	44	0,06
	14	0,99	(0,88-1,11)	236	0,04
	15	1,25	(1,19-1,39)	30	0,06
	16	1,33	(1,19-1,47)	90	0,07
	20	2,23	(1,94-2,25)	10	0,24
	21	5,15	(4,00-6,21)	19	0,49
	23	1,93	(1,85-2,07)	34	0,07
	24	0,92	(0,79-1,07)	101	0,08
	25	0,88	(0,74-1,08)	41	0,07
	26	0,87	(0,82-0,97)	136	0,05
ST_5	27	0,95	(0,89-1,10)	15	0,07
	28	0,94	(0,83-1,10)	147	0,06
	29	0,93	(0,81-1,09)	75	0,07
$ST_{6.1}$	30	0,82	(0,73-0,97)	16	0,07
	31	0,85	(0,77-0,98)	25	0,07
	32	0,99	(0,89-1,10)	106	0,05
$ST_{6.2}$	33	0,81	(0,69-0,93)	122	0,05
	34	0,77	(0,73-0,82)	11	0,04
	35	0,78	(0,70-0,86)	26	0,05

Table 3.

Randon reflectance (Rr%), range of Rr%, number of measurements and standard deviation of coal samples from borehole 2TG-227-RS, Santa Terezinha Coal Field, Rio Grande do Sul, Brazil

macrinite. Clarite is an association of desmocollinite, microsporinite and/or liptodetrinite. Durite usually presents an association of fusinite and microsporinite. Vitrinertite presents a mixture of desmocollinite, telocollinite, gelocollinite, fusinite, semifusinite, inertodetrinite, macrinite and clay, with the predominance of macerals of the vitrinite group. Duroclarite is the most frequent microlithotype among trimacerites.

Results of microlithotype and maceral analyses are presented on Tables 1 and 2 and Figures 2 and 3.

Reflectance

The vitrinite reflectance of the coal seams from borehole 2TG-227-RS varies significantly due to the occurrence of igneous intrusive rocks (Fig. 2). Table 3 presents random reflectance values, Rr% variation, number of measurements and standard deviation for each interval. Random reflectance varies from 0.71Rr% (seam ST1) to 5.15Rr% for seam ST4. Standard deviation ranges from 0.03 to 0.49 %.

On the other hand, the variation of vitrinite reflectance along the borehole 2TG-230-RS is probably due to facies changes. Random reflectance varies from 0.73 Rr% (seam ST2) to 0.92 Rr% (interval 15) and the standard deviation ranges from 0.02 to 0.09% (Table 4).

Proximate Analysis

Proximate analysis results for samples from borehole 2TG-227-RS (Table 5) present moisture values ranging from 0.63% (ST2 and ST3 seams) to 1.63% (ST3 seam). Ash contents vary from 32.95% (ST2) to 52.34% (ST5), the volatile matter from 30.41% (ST2) to 45.69% (ST4) . Fixed carbon exceeds 50% ranging from 54.31% (ST4) to 69.59% (ST2). The analysis of samples from borehole 2TG-230-RS presents similar results (Table 5).

A sample of hand-picked vitrain collected from ST1 seam (borehole 2TG-227-RS) presents the following results: 1.02% of moisture, 13.60% of ash (dry basis), 40.30% of volatile matter (daf) and 59.70% of fixed carbon (daf).

From borehole 2TG-230-RS a sample of washed coal was taken from ST4 seam for analysis. The results are the following: moisture 0.70%, ash (dry) 15%, volatile matter (daf) 36.70% and 63.35% of fixed carbon (daf).

Organic Geochemistry

Representative samples with low mineral matter content were chosen for the organic geochemistry study.

Bitumen Extraction and
Liquid Chromatooraphy

Table 6 shows bitumen extraction results. For samples from borehole 2TG-227-RS they range from 3345 ppm in ST6.1 seam to 13671 ppm in ST3 seam.

Samples from borehole 2TG-230-RS present lower contents of bitumen extract than samples from borehole 2TG-227-RS. The contents range from 2533 ppm in ST6.1 seam to 9260 ppm in the ST2 seam.

Contents of aliphatic hydrocarbons for borehole 2TG-227-RS range from 4.11 % (ST6.1 seam) to 24.89% at the top of ST4 seam, whereas for borehole 2TG-230-RS, the contents vary from 0.95% (interval 16) to 11.35% (ST6.2 seam).

Contents of aromatic hydrocarbons are usually high, ranging from 16.08% to 23.42% at the top

Seam	Sample number	Rr%	Rr% range	number of measurements	standard deviation
ST_2	1	0,76	(0,70-0,87)	62	0,03
	2	0,84	(0,77-0,93)	176	0,07
	3	0,73	(0,70-0,84)	149	0,07
	4	0,75	(0,70-0,81)	62	0,02
	5	0,78	(0,77-0,82)	100	0,08
	6	0,77	(0,74-0,82)	163	0,02
	7	0,77	(0,70-0,87)	28	0,06
ST_3	9	0,90	(0,85-0,97)	110	0,09
(ST_4)	Seam B	0,79	(0,70-0,89)	70	0,04
ST_4	10	0,86	(0,80-0,95)	168	0,09
	11	0,84	(0,74-0,94)	216	0,04
ST_5	13	0,92	(0,83-1,01)	104	0,04
	15	0,92	(0,85-1,09)	142	0,09
$ST_{6.1}$	16	0,79	(0,70-0,80)	142	0,09
	17	0,83	(0,74-0,92)	51	0,05
	18	0,86	(0,80-0,97)	52	0,05
	19	0,88	(0,80-0,97)	38	0,05
	20	0,82	(0,71-0,97)	48	0,05
$ST_{6.2}$	21	0,89	(0,80-1,00)	24	0,06

Table 4. *Randon reflectance (Rr%), range of Rr%, number of measurements and standard deviation of coal samples from borehole 2TG-230-RS, Santa Terezinha Coal Field, Rio Grande do Sul, Brazil*

SEAM	Sample Number	Moisture%	Ash (dry)%	V.Matter (d.a.f.)%	F. Carbon%
		Borehole 2-TG-227-RS			
ST1	1	0.64	36.02	40.87	59.13
ST2	7	0.63	32.95	30.41	69.59
ST3	9	1.63	37.08	34.16	65.84
	10	0.69	43.72	34.86	65.14
ST4	14	0.63	37.78	37.11	62.83
	24	1.34	53.91	31.43	68.57
	26	0.82	34.05	45.69	54.31
ST5	28	1.23	52.34	37.24	62.76
ST6.1	32	0.94	48.30	34.09	65.97
		Borehole 2-TG-230-RS			
ST2	3	0.65	44.36	45.29	54.71
	5	0.79	52.53	47.94	54.39
	6	0.8	51.5	47.1	52.9
ST4	10	0.9	32.03	37.59	63.95
	11	0.87	26.64	32.26	63.72
ST5	13	1	44.16	38.27	61.71
ST6.1	16	0.52	56.88	37.32	67.68
	17	0.61	56.81	37.19	62.81
	18	0.32	40.01	33.82	66.18
	20	0.65	34.73	34.31	65.68
ST6.2	21	0.73	43.17	39.16	60.84

Table 5. *Results of proximate analysis of samples from boreholes 2TG-227-RS e 2TG-230-RS, Santa Terezinha Coal Field, Rio Grabde do Sul, Brazil.*

Seam	Sample number	Bitumen Extract (ppm)	Aliphatics %	Aromatics %	NSO %	Pr/Ph	Pr/n-C17	Ph/n-C18	CPI
Borehole 2-TG-227-RS									
ST1	1	6829.41	7.7	23.5	68.8	7.4	1.8	0.3	
ST2	7	8293.61	17.6	38.1	44.3	4.3	1.3	0.3	1.01
ST3	9	13671.0	8.1	23.4	68.5	4.6	2.0	0.4	1.02
	10	5202.5	15.6	30.9	53.5	5.0	1.4	0.3	1.02
ST4	14	8898.43	21.9	30.8	47.4	3.7	0.6	0.2	1.01
	24	5823.27	15.2	41.3	43.5	3.9	0.4	0.1	
	26	5308.0	11.4	25.2	63.4	6.3	0.8	0.1	
ST5	28	3985.45	6.6	22.8	70.7	4.2	0.9	0.2	0.98
ST6.1	32	3345.0	4.1	16.1	79.8	1.9	0.8	0.2	0.96
Borehole 2-TG-230-RS									
ST2	3	9260.0	7.6	29.7	62.7	6.7	4.8	0.8	1.15
	5	6670.0	4	23.5	72.5	5.2	3.7	0.6	1.11
	6	8209.52	0.95	22.2	76.8	2.7	2.4	0.4	1.14
ST4	10	6307.69	10.7	28.1	61.3	5.9	3.1	0.5	1.12
	11	8954.54	9.5	22.5	68.0	4.7	1.8	0.3	1.10
ST5	13	6032.07	10.6	30.8	58.6	6.5	1.9	0.3	1.08
	16	2533.33	7.2	17.1	75.7	2.5	0.6	0.2	1.11
ST6.1	17	4506.25	9.1	23.1	67.7	3.2	1.0	0.3	1.14
	18	5425.64	9.6	27.8	62.6	3.9	1.1	0.3	1.14
	20	7878.94	10.5	21.7	67.8	5.4	1.8	0.3	1.09
ST6.2	21	9228.0	11.4	28.6	60.1	7.4	6.3	0.9	1.13

Table 6. *Results of bitumen extract (ppm), Aliphatics %, Aromatics %, NSO %, Pristane / Phytane (Pr / Ph), Pr / n-C_{17} , Ph / n-C_{18} and CPI of samples from boreholes 2TG-227-RS and 2TG-230-RS.*

of ST3 seam for the samples from borehole 2TG-227-RS. As for borehole 2TG-230-RS, the samples present aromatic hydrocarbon contents varying from 17.12% at the top of ST6.1 seam to 29.2% at the top of ST2.

Among the studied fractions, NSO compounds are the most abundant for both sections, ranging from 43.52% at the bottom of ST4 seam (2TG-227-RS) to 76.81% (interval 16 - 2TG-230-RS; Table 6).

Geochemical Molecular Indicators

The chromatograms of saturated hydrocarbons (aliphatics) display n-alkanes extending up to n-C_{29}. Samples from 2TG-227-RS present a predominance of C_{17} to C_{21} while samples from 2TG-230-RS show a predominance around C_{23} and a slight predominance of even-numbered n-alkanes (Figs. 4 and 5). The abundance of n-C_{17} to n-C_{20} is related to the hydrocarbon composition of algae and

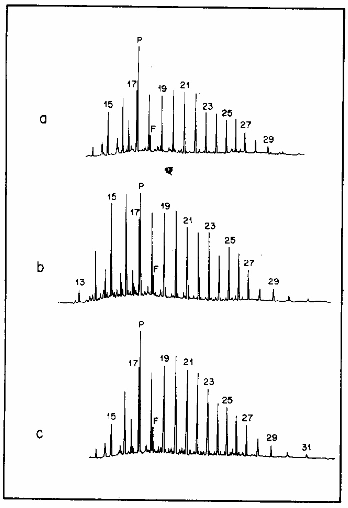


Figure 4. *Gas chromatograms of saturated hydrocarbons of coal extracts of the following intervals: a) ST1 (sample 1); b) ST2 (sample 7) and c) ST3 (sample 9) of 2TG-227-RS borehole.*

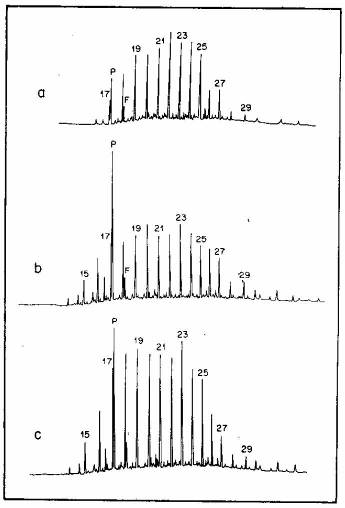


Figure 5. *Gas chromatograms of saturated hydrocarbons of coal extracts of the following intervals: a) sample 6; b) ST4 (sample 10) and c) sample 11, of 2TG-230-RS borehole.*

phytoplancton and the long-chain components (more than C_{20}) are related to higher terrestrial plant input. Mukwopadhyay et al. (1979) observed in some coal basins in India a smooth rise and decline of peaks from n-C_{15} to n-C_{25} and predominance of higher homologues (more than C_{20}) in the lower coalification stage and a predominance of lower homologues (below n-C_{20}) in the higher coalification stage. Among the hydrocarbon isoprenoids only pristane and phytane were identified. Table 6 presents the ratios of pristane/phytane (Pr/Ph), pristane/n-C_{17} (Pr/n-C_{17}), phytane/n-C_{18} (Ph/n-C_{18}), and carbon preference index (CPI)[2] for 2TG-227-RS and

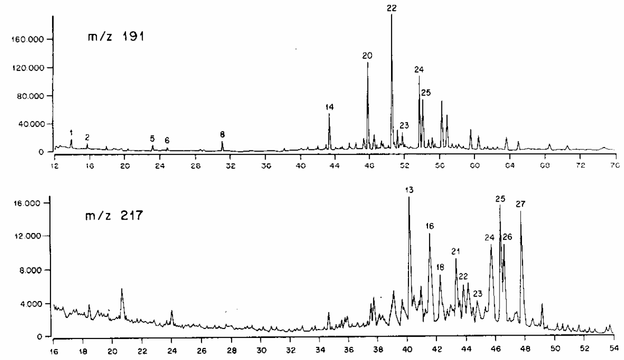
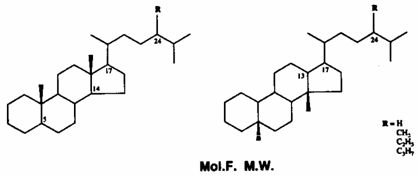


Figure 6. *m/z fragmentograms of the satured fractions from coal extracts. m/z 191 (terpanes) and m/z 217 (steranes) of sample 1 of ST1 seam from 2TG-227-RS borehole.*

STERANES

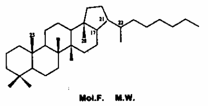


R = H C_{27}
CH_3 C_{28}
C_2H_5 C_{29}
C_3H_7 C_{30}

Steranes

		Mol.F.	M.W.
1 -	13β(H),17α(H)-Diacholestane (20S)	$C_{27}H_{48}$	372
2 -	13β(H),17α(H)-Diacholestane (20R)	$C_{27}H_{48}$	372
3 -	13α(H),17β(H)-Diacholestane (20S)	$C_{27}H_{48}$	372
4 -	13α(H),17β(H)-Diacholestane (20R)	$C_{27}H_{48}$	372
5 -	13β(H),17α(H),24-methyl-Diacholestane (20S)	$C_{28}H_{50}$	386
6 -	24R/S isomers		
7 -	n.d.		
8 -	n.d.		
9 -	13β(H),17α(H),24-methyl-Diacholestane (20R)	$C_{28}H_{50}$	386
10 -	24R/S isomers		
11 -	13α(H),17β(H),24-methyl-Diacholestane (20S)	$C_{28}H_{50}$	386
12 -	5α(H),14α(H),17α(H)-Cholestane (20S)	$C_{27}H_{48}$	372
13 -	5α(H),14β(H),17β(H)-Cholestane (20R) +	$C_{27}H_{48}$	372
	13β(H),17α(H),24-ethyl-Diacholestane (20S)	$C_{29}H_{52}$	400
14 -	5α(H),14β(H),17β(H)-Cholestane (20S) +	$C_{27}H_{48}$	372
	13α(H),17β(H),24-methyl-Diacholestane (20R)	$C_{28}H_{50}$	386
15 -	5α(H),14α(H),17α(H)-Cholestane (20R)	$C_{27}H_{48}$	372
16 -	13β(H),17α(H),24-ethyl-Diacholestane (20R)	$C_{29}H_{52}$	400
17 -	n.d.		
18 -	13α(H),17β(H),24-ethyl-Diacolestane (20S)	$C_{29}H_{52}$	400
19 -	n.d.		
20 -	5α(H),14α(H),17α(H),24-methyl-Cholestane (20S)	$C_{28}H_{50}$	386
21 -	5α(H),14β(H),17β(H),24-methyl-Cholestane (20R) +	$C_{28}H_{50}$	386
	13α(H),17β(H),24-ethyl-Diacholestane (20R)	$C_{29}H_{52}$	400
22 -	5α(H),14β(H),17β(H),24-methyl-Cholestane (20S)	$C_{28}H_{50}$	386
23 -	5α(H),14α(H),17α(H),24-methyl-Cholestane (20R)	$C_{28}H_{50}$	386
24 -	5α(H),14α(H),17α(H),24-ethyl-Cholestane (20S)	$C_{29}H_{52}$	400
25 -	5α(H),14β(H),17β(H),24-ethyl-Cholestane (20R)	$C_{29}H_{52}$	400
26 -	5α(H),14β(H),17β(H),24-ethyl-Cholestane (20S)	$C_{29}H_{52}$	400
27 -	5α(H),14α(H),17α(H),24-ethyl-Cholestane (20R)	$C_{29}H_{52}$	400

TERPANES



Terpanes

		Mol.F.	M.W.
1 -	C_{19} Tricyclic terpane	$C_{19}H_{34}$	262
2 -	C_{20} Tricyclic terpane	$C_{20}H_{36}$	276
3 -	C_{21} Tricyclic terpane	$C_{21}H_{38}$	290
4 -	C_{22} Tricyclic terpane	$C_{22}H_{40}$	304
5 -	C_{23} Tricyclic terpane	$C_{23}H_{42}$	318
6 -	C_{24} Tricyclic terpane	$C_{24}H_{44}$	332
7 -	C_{25} Tricyclic terpane	$C_{25}H_{46}$	346
8 -	C_{24} Tetracyclic terpane	$C_{24}H_{42}$	330
9 -	C_{26} Tricyclic terpane (S/R)	$C_{26}H_{48}$	360
10 -	C_{28} Tricyclic terpane (S/R)	$C_{28}H_{52}$	388
11 -	C_{29} Tricyclic terpane (S/R)	$C_{29}H_{54}$	402
12 -	18α(H),22,29,30-Trisnorneohopane (Ts)	$C_{27}H_{46}$	370
13 -	17α(H),18α(H),21β(H),25,28,30-Trisnorhopane	$C_{27}H_{46}$	370
14 -	17α(H),22,29,30-Trisnorhopane (Tm)	$C_{27}H_{46}$	370
15 -	17β(H),18α(H),21α(H),25,28,30-Trisnormoretane	$C_{27}H_{46}$	370
16 -	17β(H),22,29,30-Trisnorhopane	$C_{27}H_{46}$	370
17 -	17α(H) - demethylated Hopane (C_{28})	$C_{28}H_{48}$	384
18 -	17α(H),18α(H),21β(H),28,30-Bisnorhopane	$C_{28}H_{48}$	384
19 -	17α(H) - demethylated Hopane (C_{29})	$C_{29}H_{50}$	398
20 -	17α(H),21β(H),30-Norhopane	$C_{29}H_{50}$	398
21 -	17β(H),21α(H),30-Normoretane	$C_{29}H_{50}$	398
22 -	17α(H),21β(H)-Hopane	$C_{30}H_{52}$	412
23 -	17β(H),21α(H)-Moretane	$C_{30}H_{52}$	412
24 -	17α(H),21β(H)-Homohopane (22S)	$C_{31}H_{54}$	426
25 -	17α(H),21β(H)-Homohopane (22R)	$C_{31}H_{54}$	426
26 -	Gammacerane	$C_{30}H_{52}$	412
27 -	17β(H),21α(H)-Homomoretane	$C_{31}H_{54}$	426
28 -	17α(H),21β(H)-Bishomohopane (22S)	$C_{32}H_{56}$	440
29 -	17α(H),21β(H)-Bishomohopane (22R)	$C_{32}H_{56}$	440
30 -	17β(H),21α(H)-Bishomomoretane	$C_{32}H_{56}$	440
31 -	17α(H),21β(H)-Trishomohopane (22S)	$C_{33}H_{58}$	454
32 -	17α(H),21β(H)-Trishomohopane (22R)	$C_{33}H_{58}$	454
33 -	17β(H),21α(H)-Trishomomoretane	$C_{33}H_{58}$	454
34 -	17α(H),21β(H)-Tetrakishomohopane (22S)	$C_{34}H_{60}$	468
35 -	17α(H),21β(H)-Tetrakishomohopane (22R)	$C_{34}H_{60}$	468
36 -	17β(H),21α(H)-Tetrakishomomoretane	$C_{34}H_{60}$	468
37 -	17α(H),21β(H)-Pentakishomohopane (22S)	$C_{35}H_{62}$	482
38 -	17α(H),21β(H)-Pentakishomohopane (22R)	$C_{35}H_{62}$	482
39 -	17β(H),21α(H)-Pentakishomomoretane	$C_{35}H_{62}$	482

---

[2] The formula for calculating the Carbon Preference Index (CPI) [16.32] is:

$$\mathrm{CPI} = \frac{1}{2}\left[\frac{(17+19+21+23+25+27+29+31)}{(16+18+20+22+24+26+28+30+32)} + \frac{(17+19+21+23+25+27+29+31)}{(18+20+22+24+26+28+30+32)}\right]$$

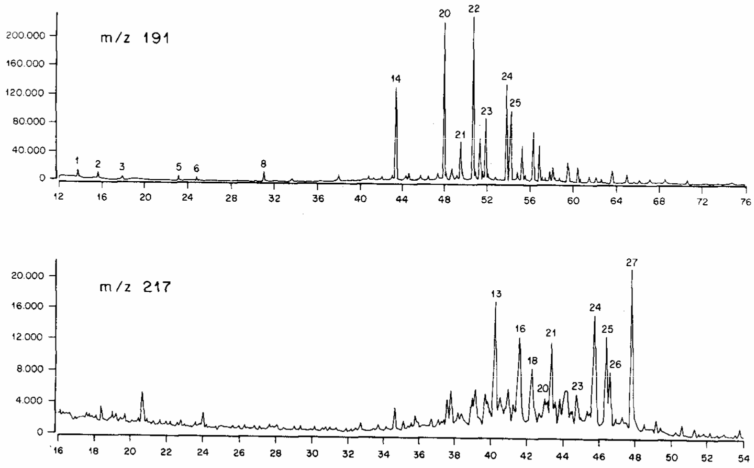


Figure 7. *m/z fragmentograms of the satured fractions from coal extracts. m/z 191 (terpanes) and m/z 217 (steranes) of sample 3 of ST2 seam from 2TG-230-RS borehole.*

2TG-230-RS boreholes.

ST6.1, ST5 and ST4 seams present Pr/n-C_{17} ratios lower than 1, whereas the other seams present values higher than 1. Ph/n-C_{18} ratios are lower than 1 for all seams and CPI varies along the whole section presenting values close to 1 (Table 6; Fig. 4).

For borehole 2TG-230-RS, Pr/Ph ratios vary from 2.5 at the top of ST6.2 seam to 7.4 (ST6.1 seam). Pr/n-C_{17} ratios are rather heterogeneous along the section, it ranges from 0.6 at the top of ST6.1 seam to 6.3 (ST6.2 seam). Ph/n-C_{18} ratios present smaller variation and values lower than 1. The Carbon Preference Index (CPI) presents values ranging from 1.08 (ST5 seam) to 1.15 at the top of ST2 seam (Table 6; Fig. 5). Pristane/phytane ratios vary between 1.9 (ST6.1 seam) and 7.4 (ST1 seam) for borehole 2TG-227-RS. Anomalously low values can be due to losses in the chromatrographic column.

The m/z 191 fragmentograms show the presence of C_{19} and C_{20} tricyclic (1 and 2), C_{24} tetracyclic terpanes (8) in all seams, reflecting an input of terrestrially derived organic matter (Abdullah et al, 1988). Samples show a high relative abundance of C_{30}-hopane (22), norhopane (20), βα hopanes (21,23) and very low Ts (12)/Tm (14) ratio (Figs. 6 and 7).

The m/z 217 fragmentograms show low diasteranes in relation to steranes (Figs.6 and 7). The GC-MS-MS data show the predominance of C_{29} over C_{27} and C_{28} steranes (Figs. 8 and 9), a

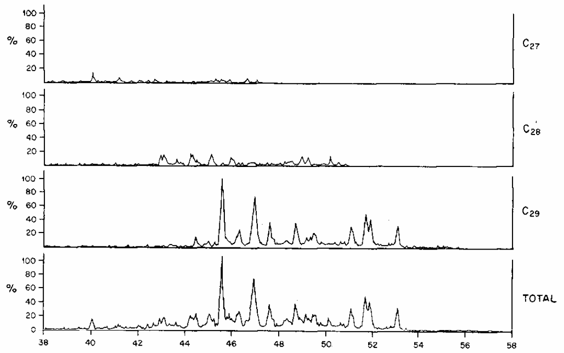


Figure 8. *GC-MS-MS fragmentograms of the saturated fractions from coal extracts separating C_{27}, C_{28} and C_{29} steranes of sample 1 (ST1 seam) of 2TG-277-RS.*

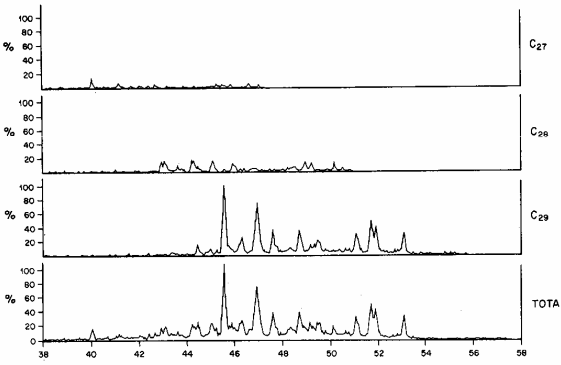


Figure 9. *GC-MS-MS fragmentograms of the saturated fraction from coal extract separating C_{27}, C_{28} and C_{29} steranes of sample 3 (ST2 seam) of 2TG-277-RS.*

distinguishing feature of terrestrially derived material, as well as a low sterane/hopane ratio (<0.1; Peters & Moldowan, 1993).

Table 7 presents selected biomarker parameters for organic matter input and maturation. For terpane ratios it is possible to observe that the average ratios are higher for 2TG-230-RS borehole. The tetracyclics/tricyclic (C_{19}-C_{20}) ranges from 0.5 to 5.1 for 2TG-227-RS borehole and from 2.0 to 8.4 for 2TG-230-RS borehole. As trisnorhopane (Ts) is almost absent in all samples and trisnorneohopane (Tm) is abundant in all samples, the ratio Tm/hopane was proposed as a maturation parameter. Sample from 2TG-227-RS borehole present very low ratios (0.2-0.3) while in 2TG-230-RS this ratio ranges from 0.5 to 0.9, pointing out to a lower maturation stage. Norhopane/hopane ratios vary between 0.5 and 0.9 for 2TG227-RS and between 0.7 and 1.4 for 2TG-230-RS. Hopane and βα hopane (moretane) are formed during diagenesis decreasing rapidly during catagenesis (Peters & Moldowan, 1993). Studies on carboniferous coals (Ten Haven et al., 1992) indicate that moretane/hopane ratios are controlled by differing rates of destruction of the isomers. Moretane/hopane ratios (around 0.1) for 2TG-227-RS are equivalent to those typical for mature source rocks. The ratio of αββ/(αββ + ααα) of the C_{29} regular sterane seems to be a maturation parameter independent of source input (Peters & Moldowan, 1993). An increase of this ratio is caused by isomerization at the C-14 and C-17 positions in the 20S and 20R C_{29} regular steranes.

Borehole 2-TG-227-RS		Terpanes				Steranes
Seam	Sample number	Tetrac/Tricyclics	Tm/Hopane	Norhop/Hop	Moretane/Hop	C29abb/abb+aaa
ST1	1	2	0.3	0.7	0.1	0.51
ST2	7	0.5	0.3	0.6	0.1	0.56
ST3	9	0.5	0.3	0.7	0.1	0.49
	10	3.0	0.3	0.6	0.1	0.53
ST4	14		0.2	0.5	0.1	0.46
	24	4.5	0.2	0.5	0.1	0.49
	26	4.7	0.3	0.6	0.1	0.45
ST5	28	5.1	0.3	0.6	0.1	0.46
ST6.1	32	3.9	0.3	0.9	0.1	0.47
Borehole 2-TG-230-RS						
ST2	3	2.4	0.6	1.0	0.4	0.34
	5	2.1	0.5	0.8	0.3	0.36
	6	2.2	0.6	0.9	0.3	0.35
ST4	10	5.2	0.6	0.7	0.4	0.32
	11	5.5	0.7	0.7	0.4	0.34
ST5	13	8.4	0.8	0.8	0.5	0.32
	16	5.2	0.9	1.0	0.5	0.28
ST6.1	17	4.2	0.7	1.4	0.5	0.32
	18	8.3	0.7	1.4	1.5	0.33
	20	2.0	0.7	1.2	0.5	0.31
ST6.2	21	4.1	0.6	1.1	0.3	0.38

Table 7. *Some biomarker parameters for input and maturation interpretation of samples from boreholes 2TG-227-RS and 2TG-230-RS*

Borehole 2-TG-227-RS								
Seam	Sample number	Norhop/Hop	Vitrinite%	Inertinite%	Liptinite%	Rr%	$\delta^{13}C$ ‰ (PDB)	Groups of samples
ST1	1	0.7	90.3	7.6	2.1	0.71	(-25.0)	A
ST2	7	0.6	90.2	9.6	0.2	0.91	(-24.9)	A
ST3	9	0.7	90.2	8.4	1.4	0.81	(-24.7)	A
	10	0.6	89.0	8.3	2.7	0.80	(-24.6)	A
ST4	14	0.5	77.9	21.2	0.8	0.99	(-24.0)	B
	24	0.5	42.2	53.8	4.0	0.92	(-23.3)	B
	26	0.6	78.2	13.4	8.4	0.87	(-21.7)	B
ST5	28	0.6	63.1	29.7	7.2	0.94	(-22.6)	B
ST6.1	32	0.9	30.6	56.1	13.3	0.99	(-23.9)	C
Borehole 2-TG-230-RS								
ST2	3	1.0	86.5	7.8	5.7	0.73	(-24.7)	A
	5	0.8	91.2	7.8	1.0	0.78	(-24.6)	A
	6	0.9	88.7	10.3	1.0	0.77	(-24.7)	A
ST4	10	0.7	57.7	30.4	11.8	0.86	(-22.6)	B
	11	0.7	72.0	24.3	3.7	0.84	(-23.5)	B
ST5	13	0.8	47.7	38.9	13.4	0.92	(-22.9)	B
	16	1.0	81.2	16.2	2.6	0.79	(-22.1)	B
ST6.1	17	1.4	12.8	74.6	12.6	0.83	(-21.7)	C
	18	1.4	19.9	64.3	15.8	0.86	(-21.5)	C
	20	1.2	18.6	69.8	11.6	0.82	(-22.1)	C
ST6.2	21	1.1	8.6	79.6	11.8	0.89	(-23.6)	C*

Table 8. *Some geogemichal and petrological parameters for characterization of groups of samples from boreholes 2TG-227-RS and 2TG-230-RS*

A ratio of about 0.7 indicates that this reaction reaches equilibrium (Seifert & Moldowan, 1986). The ratios obtained for the Santa Terezinha coal samples are lower than 0.7, varying from 0.46 to 0.56 in 2TG-227-RS borehole and from 0.28 to 0.38 in 2TG-230-RS borehole (Table 7). These values do not correlate well with the mean vitrinite reflectance (Table 8) obtained but, nevertheless, indicate that samples of 2TG-227-RS were submitted to a higher thermal stress than the samples collected from 2TG-230-RS.

Isotopic Analysis

The carbon isotopic analysis were carried out according to an international standard (Belemnite of Pee Dee Formation, Upper Cretaceous, South Carolina).

For borehole 2TG-227-RS, the carbon isotopic values vary between -21.7‰ at the bottom of ST4 seam and -25.0‰ (ST 1 seam), whereas for borehole 2TG-230RS the values range from - 21.59 at the top of ST6.1 to -24.7‰ at the top of ST2 seam and interval 6 (Table 8).

DISCUSSION

Rank

Random reflectance, moisture and volatile matter contents of hand picked vitrain were considered for rank determination of the coal seams, according to German (DIN) and American (ASTM) classifications.

The values of Rr% obtained for samples from borehole 2TG-227-RS, including those intervals associated with intrusive bodies, allowed their classification as Flammkohle/Gasflammkohle, corresponding to the stage of High Volatile Bituminous B coal, to Magerkohle, corresponding to the stage of Semi Anthracite, in the case of seams ST2 and ST4, affected by igneous intrusive rocks (Table 9).

Fluctuations in random reflectance with depth (Figs. 2 and 3), disregarding the variation caused by intrusive bodies, are consistent with rank studies carried out for several coal fields in Brazil. Corrêa da Silva & Wolf (1980) analysed the coal seams of Harmonia (Paraná State), Irapuá (Santa Catarina State) and Morungava (Rio Grande do Sul State) and observed a large variation of Rr% values with depth and suggested that it was caused by the influence of roof sandstones, maceral composition or the sapropelic character of these coals.

Souza Lima (1984) observed in coals from Chico Lomã Coalfield, near Santa Terezinha (Fig. 1), that vitrinite reflectance varies largely from one seam to another within a thickness of about 28 m.

The rank determined on the basis of vitrinite reflectance, volatile matter (daf) and moisture of hand picked vitrain of ST1 seam (borehole 2TG-227-RS) and vitrinite reflectance, volatile matter (daf) and moisture of the fraction floated on liquid with density -1.50 of ST4 seam (borehole 2TG-230-RS), both with about 14% ash (dry basis) showed a good correlation among these parameters. The coals of ST1 seam were classified

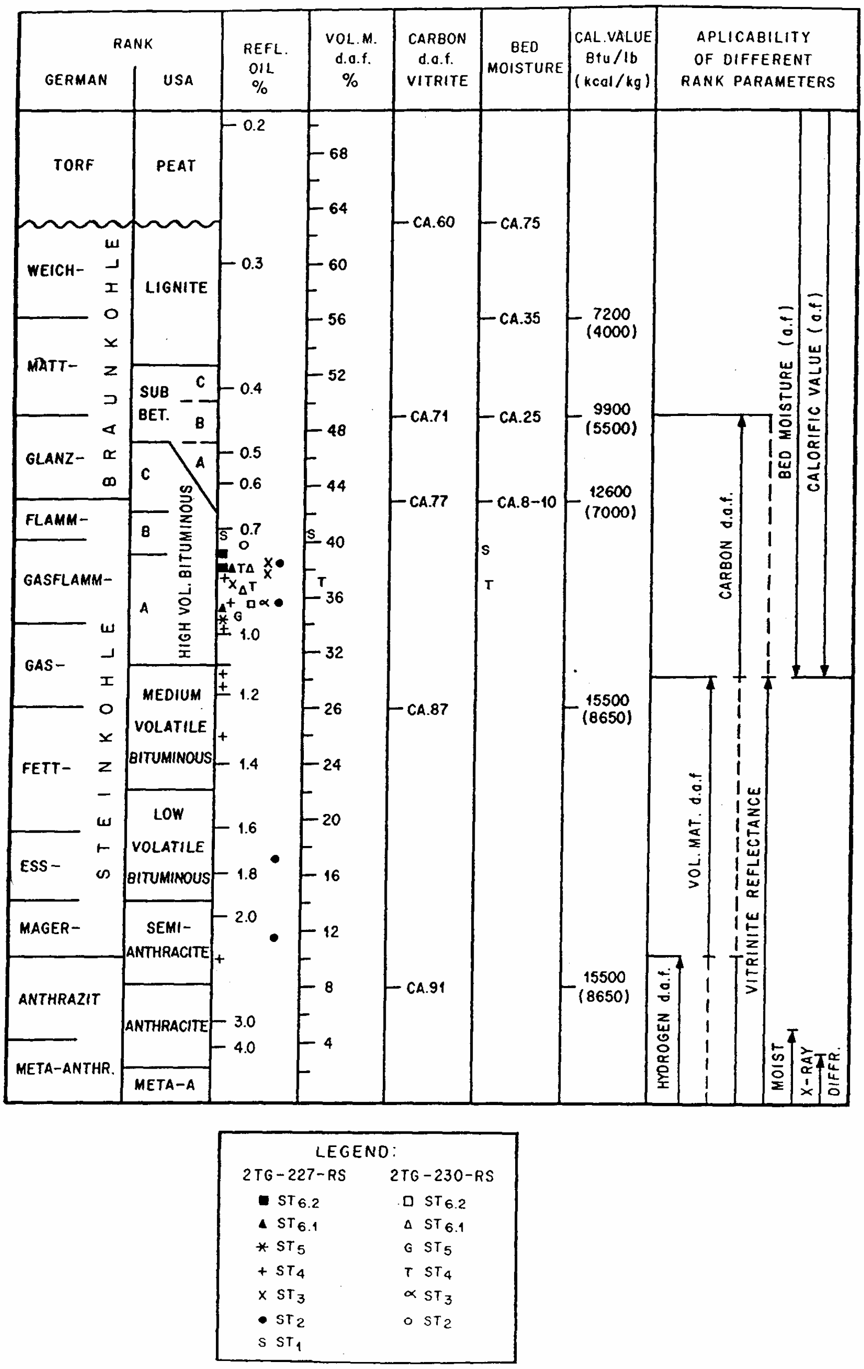


Table 9. *Coalification stage according to DIN and ASTM classifications. Simbols plotted in the table correspond to the studied samples from boreholes 2TG-227-RS and 2TG-230-RS*

as High Volatile Bituminous B Coal and of ST4 seam as High Volatile Bituminous A Coal.

Although, in terms of rank evaluation, the samples from 2TG-227-RS present a good correlation between moisture content (%) and carbon preference index (CPI), samples from borehole 2TG-230-RS show values of moisture lower than it would be expected taken into account other rank parameters such as CPI and Rr%.

The general maturation trend presented by the studied coals suggests an internal variation of coalification, from bottom to top, and an increase of rank eastwards.

The higher contents of bitumen extracts (Table 6) are, in general, related to high vitrinite reflectance values as well as to the percentage of aliphatic compounds. It was observed by Durand et al.,1977 (in Tissot & Welte, 1978) that extracts increased to a maximum in High Volatile Bituminous Coals with corresponding to vitrinite reflectance values of 0.8 to 1.0 Ro%. Besides maturation effects high values (ppm) of bitumen extracts could also be related to the organic composition. Mukwopadhyay et al. (1979) observed that the content of extracts in coals from India was related to the nature of liptinitic macerals and to rank.

Coal Composition

The composition of the studied coals, disregarding mineral matter contents, is shown on Tables 10 and 11 and Figure 10. This figure shows that the contents of inertinite are usually high (more than 30%), the rate of vitrinite is variable and the contents of liptinite are low. Nevertheless, the gas chromatograms of seams ST1, ST2 and ST3 of borehole 2TG-227-RS (Fig.4) point out the presence of alginite. The underestimation of liptinite macerals in combined analysis could be due to the close association between these macerals and mineral matter since it was done under white light.

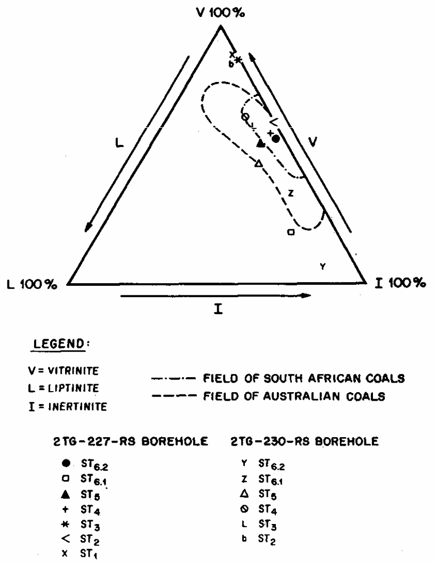


Figure 10. *Triangular compositional plot of maceral groups (without mineral matter) of the studied samples from boreholes 2TG-227-RS and 2TG-230-RS. Fields of Gondwana coals according to Mackowsky (1975).*

Although the average petrographic composition of each seam show a scattered distribution on the maceral composition ternary diagram, it is possible to observe a tendency to be plotted inside the field of Gondwana coals (in the sense of Mackowsky, 1975).

ST6.2 seam (borehole 2TG-230-RS) and ST6.1 seam (borehole 2TG-227-RS) were plotted outside the field of Gondwana coals due to their high contents of inertinite (higher than 50%) and amounts of liptinite (about 15%) slightly higher than the average.

ST1 and ST3 seams (borehole 2TG-227-RS) and ST2 seam (2TG-230-RS) were plotted

Seams	Vitrinite%	Liptinite%	Inertinite%
ST1	90	2	8
ST2	63		37
ST3	88	2	10
ST4	58	4	38
ST5	55	9	36
ST6.1	20	15	65
ST6.2	58	3	39

Table 10. *Maceral groups percentage (excluding mineral matter contents). Seam composition was calculated from avarage percentage of each interval, borehole 2TG-227-RS*

Seams	Vitrinite%	Liptinite%	Inertinite%
ST2	86	4	10
ST3(botton)	61	9	30
ST4	65	9	26
ST5(botton)	48	13	38
ST6.1	34	10	56
ST6.2	7	11	81

Table 11. *Maceral groups percentage (excluding mineral matter contents). Seam composition was calculated from avarage percentage of each interval, borehole 2TG-230-RS*

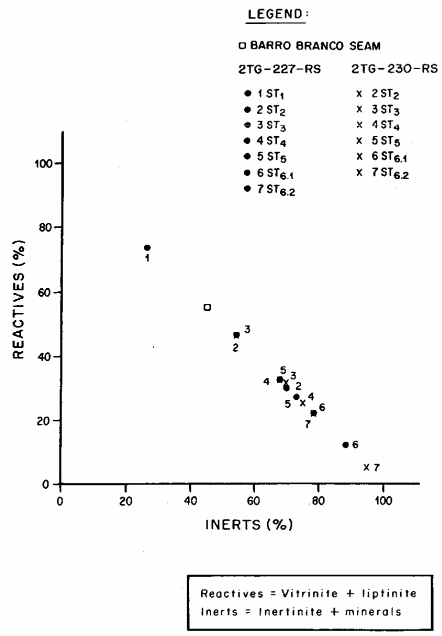


Figure 11. *Reactives X Inerts diagram of the studied samples from boreholes 2TG-227-RS and 2TG-230-RS and of the Barro Branco seam.*

outside the field of Gondwanic coals (South Africa and Australia) because of their very high vitrinite average contents. The maceral composition of these coals is comparable to some European coals (Corrêa da Silva & Wolf, 1980).

Figure 11 shows that in the majority of the seams the contents of reactives (vitrinite+inertinite) are, in general, less than 30%. Only ST3 seam (2TG-227-RS) and ST2 seam (2TG-230-RS) approach the representative point of the Barro Branco Seam (Santa Catarina). ST1 seam (2TG-227-RS) is the richest seam in reactives (nearly 76%) and presents only 24% of inerts (inertinite+mineral matter).

According to Matos & Souza Lima (1984) reactives (vitrinite+liptinite) are also low for coals from Chico Lomã Coalfield because of the high contents of mineral matter in these coals.

Organic facies

According to Teichmuller & Teichmuller (in Stach et al. 1982) the term coal facies refers to the primary genetic types of coal, which are dependent on the depositional environment under which the peat originated.

The facies of the coal seams is directly related to the depositional environment, which includes kind of deposition (alochthonous or autochthonous), environment of deposition (telmatic, limnic-telmatic, etc.), peat-forming plant community, pH conditions, temperature, sulphur supply, and so on. Therefore, the maceral and mineral contents of a given sample reflect the association of these aspects.

Based on the organic composition of coals, Oswald (1937, in: Hacquebard & Donaldson, 1969) proposes a subdivision of depositional coal basins into three zones, according to water level variation:

- Terrestrial Zone: above high water level;
- Telmatic Zone: between high and low water levels;
- Limnic Zone: below low water level.

The diagram of Hacquebard & Donaldson (1969) was used for facies study of the coal seams of Santa Terezinha Coalfield. The original diagram was modified and the apices now stand

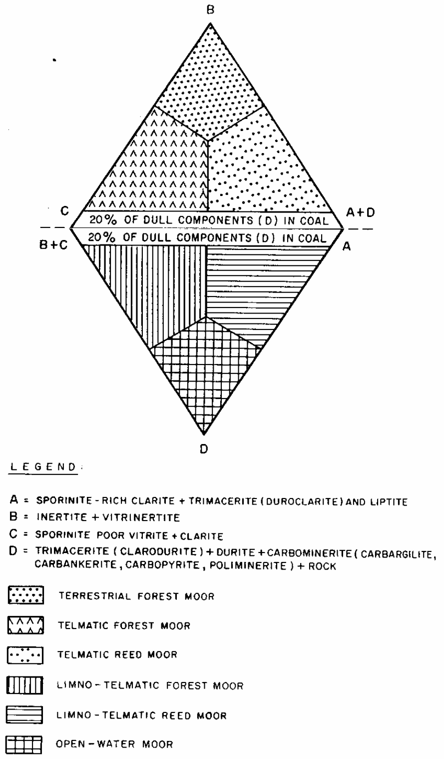


Figure 12. *Facies diagram modified from Hacquebard & Donaldson (1969)*

for the following associations (Fig. 12):

- A - sporinite-rich clarite + trimacerite (duroclarite) and liptinite
- B - inertite + vitrinertite
- C - trimacerite + sporinite-poor clarite
- D - trimacerite (clarodurite) + durite + carbominerite (carbargilite + carbopyrite + carbankerite) + rock.

There is a predominance of the open moor facies for the deposition of Santa Terezinha coal seams. The large amount of mineral matter, which reflects the association carbominerite + rock, shows an essentially subaquatic deposition. As for borehole 2TG-227-RS, it can be said that deposition started under dominant limnic conditions owing to the carbominerite + rock association (ST6.2 and ST6. 1 seams).

The first signs of depositional facies changes can be noticed at the bottom of ST4 seam, where there is a predominance of a limno-telmatic forest moor facies. Such a change reflects the decrease of the carbominerite + rock association and the importance of the B + C association (inertinite + vitrite + sporinite-poor trimacerite). It is possible to observe the variation of water table along the section, it becomes thicker in the central portion of ST4 seam and towards the top of this seam the water turns to be shallow again with the change to a limno-telmatic forest moor facies. Although these variations in water table can be noticed, ST3 and ST2 seams were deposited in a predominantly open moor facies. Another evidence of deposition under dominant subaquatic conditions is the predominance of low molecular weight hydrocarbons (C_{15}- C_{17}) derived mainly from algae (Tissot & Welte, 1978). This feature is well developed by sample 7 from ST2 seam (Fig.4,b).

Drastic facies changes can be observed towards the top of the section. ST1 seam presents a significant decrease of the carbominerite + rock association, a significant increase of the B + C association and high contents of vitrite. These changes indicate a return to limno-telmatic forest moor conditions.

Souza Lima (1984) observed that coals from Chico Lomã Coalfield (borehole 2TG-88-RS) also presents water level variation. At the lower seams limnic and limno-telmatic facies are interbedded. The seams of the middle portion present telmatic facies and limno-telmatic facies at the top.

Coal seams from Morungava Coalfield, which is located near Chico Lomã and Santa Terezinha coal fields (Fig.1) were characterized mostly as limnic with marginal vegetation and relatively fast subsidence by Corrêa da Silva (1981).

Comparison between the two boreholes and with other coals

The results of the organo-geochemical analyses indicate significant variations in maceral composition and coal rank. Several geochemical parameters used to determine the rank and organic facies vary in the two boreholes.

The results of liquid chromatography show a tendency of the samples from borehole 2TG-227-RS to shift towards the aliphatic hydrocarbons as a consequence of a higher degree of coalification (Fig. 13).

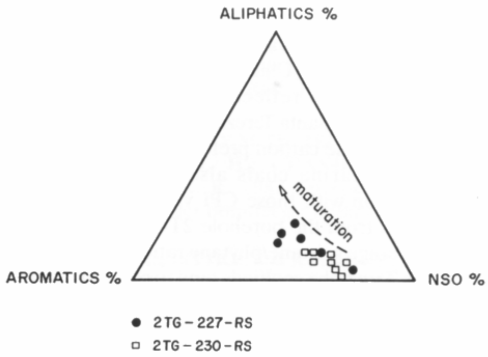


Figure 13. *Triangular plot showing relative proportions of saturated hydrocarbons (aliphatics), aromatic hydrocarbons and NSO compounds (Res + Asf) of the studied samples from boreholes 2TG-227-RS and 2TG-230-RS.*

Pristane/Phytane, Pr/n-C_{17} and Ph/n-C_{18} ratios as well as CPI point out that the samples from borehole 2TG-227-RS reached a higher stage of maturation if compared to those from 2TG-230-RS.

Terpane analysis evidenced that the coals from borehole 2TG-230-RS are richer in tetracyclics in relation to tricyclics (C_{19}, C_{20}), Trisnorhopane (Tm)/hopane (C_{30}), norhopane/hopane (C_{30}), moretane/hopane (C_{30}) ratios are higher for 2TG-230-RS and ($\alpha\beta\beta/\alpha\alpha\alpha$ + $\alpha\beta\beta$) C_{29} regular steranes ratios are higher for 2TG-227-RS pointing out a higher maturation for samples from this borehole (Table 7).

Tables 12 and 13 present some petrographic and geochemical analyses of samples from Chico Lomã (Corrêa da Silva et al., 1987) and Santa Catarina Coalfields (Püttmann et al., 1986) accordingly, in order to observe if there is any

Seam	Rr%	Vitrinite% *	Liptinite% *	Inertinite% *	TOC%	B.Extract(ppm)	CPI	P/F	P/n-C17
C.Lomã 2	0.61	54	17	29	50.9	8179	1.19	8.14	4.32
C.Lomã 4	0.69	43	16	41	40.9	11987	1.18	8.14	3.68
C.Lomã 6	0.67	64	4	32	30.6	7065	1.11	7.82	4.52

Table 12. *Petrological and geochemical results of some coal seams from Chico Lomã coal field modified from Corrêa da Silva et al. 1987 (* percentages without mineral matter content)*

Coal Sample	Rr%	Vitrinite%	Liptinite%	Inertinite%	Sporinite%	Alginite %	Liptodetrinite%	CPI	P/F
Sta. Catarina	0.80	53	32	15	2	95	3	1.03	3.78

Table 13. *Petrological and geochemical results of a Santa Catarina coal sample modified from Pütmann et al. 1986*

regional correlation between these two coalfieds and the representative samples of Santa Terezinha area. In terms of rank it is possible to observe that samples from Chico Lomã present an average lower vitrinite reflectance than the studied samples from Santa Terezinha and Santa Catarina coalfieds. The carbon preference index (CPI) of Santa Catarina coals also presents a good correlation with those CPI values obtained for samples from the borehole 2TG-227-RS (Table 6). Average pristane/phytane ratios of coals from Santa Terezinha coalfieds tend to correlate better to Santa Catarina than to Chico Lomã. As a matter of fact Pr/Ph and Pr/n-C_{17} higher ratios of Chico Lomã samples also provide an indication of the lower maturation reached by these coals (Tissot & Welte, 1978).

Despite the lower rank of samples from Chico Lomã coalfield the organic extracts contents (Table 12) are close to the mean values obtained for the Santa Terezinha coal samples (Table 6). Regarding maceral composition, the content of liptinite of Santa Catarina coal is much higher than the content of any seam of Santa Terezinha coalfield. Nevertheless, it is possible that the liptinite contents of Santa Terezinha samples could be underestimated due to its close association with mineral matter (Table 10 and 11).

CONCLUSIONS

The maceral composition of coals collected from the boreholes indicate four groups of samples with different composition. These groups were called A, B, C, and C*, in the case of borehole 2TG-230-RS (Table 8).

The variation of stable carbon isotope ratios shows a good correlation with groups A, B, C, and C*. Group A presents the most homogeneous and the lightest carbon isotope values. This group is characterized by the predominance of macerals of the vitrinite group and, in general, by a lower rank. Group C shows the heaviest carbon isotopic ratios for borehole 2TG-230-RS and a ratio similar to Group A for borehole 2TG-227-RS.

Groups B and C* show intermediate and less homogeneous carbon isotopic values. Group C* presents 80% of macerals of the inertinite group.

From Group C to A it is possible to observe clearly a variation of the depositional environment. This change in the organic facies is masked when mineral matter contents of each interval is taken into account.

The change from one group to another is normally marked by the progressive lowering of the water table from bottom to top.

REFERENCES

ABDULLAH, W. H.; GJELBERG, J.; JONES, J. M.; MURCHISON, D.G. & TELNAES, N. 1988 Early carboniferous coal depositional environment in Spitzbergen. In: *Advances of Organic Geochemistry*, 2:953-64.

ARAUJO, C.V. 1990 *Estudo petrográfico e geoquímico de carvões da Jazida de Santa Terezinha, Rio Grande do Sul, Brasil.* Master Thesis, Curso de Pós Graduação em Geociências, UFRGS. Unpublished.

CORREA DA SILVA,Z.C. 1981 Origin and Facies of some Brazilian Coal Seams. In: International Conference on Coal Science, Düsseldorf, 1981. *Proceedings*, p.39-43.

CORREA DA SILVA, Z.C. & MARQUES-TOIGO, M. 1975 Carvão no Brasil: Mina de Candiota, Rio Grande do Sul. In: II Congresso Ibero-Americano de Geologia Economica, Buenos Aires, 1975. *Actas*, 1:263-285.

CORRÊA DA SILVA, Z.C. PÜTTMANN, W.; WOLF, M. 1987 Studies on the rank determination of South Brazilian Gondwana coals. 1987 *International Conference on Coal Science*, J.A. Moulijn et al. Editors, p.165-68.

CORREA DA SILVA, Z.C. & WOLF, M. 1980 O poder refletor como parâmetro para determinação do grau de carbonificação dos carvões gonduanicos do Brasil. *Pesquisas*, Instituto de Geociências, UFRGS, Porto Alegre, **13**:35-42.

FABRICIO. J.A.C.:CAYE. B.R.; VOGT. E.; FERREIRA, J.A.F. & SÜFFERT, T. 1980 Projeto Carvão Gravataí-Torres. CPRM Internal Report, v.I. Unpublished.

HAQUEBARD, P.A. & DONALDSON, R. 1969 Carboniferous coal deposition associated with flood-plain and limnic environments in Nova Scotia. In. E.C.Dapples & M.E.Hopkins (Editors), Environments of Coal Deposition. Geol.Soc. Am., *Special Paper*, **114**: 143- 191.

MACKOWSKY, M.Th. 1975 Comparative petrography of Gondwana and Northern Hemisphere coals related to their origin. In: Campbell Ed., *3rd Gondwana Symposium*, Canberra, Australia, 1973.p.195-220.

MATOS,L.C.& SOUZA LIMA,L.M.F. 1984 Estudo petrográfico dos carvões da sondagem TG-88-RS, Jazida de Chico Lomã, RS. In: Congresso Brasileiro de Geologia, 32.*Anais*, Rio de Janeiro, SBG, **3**:1314-1319.

MUKHOPADHYAY, P.K.; HAGEMANN, H.W.; HOLLERBACH, A. & WELTE, D.H. 1979 The relation between organic geochemical and petrological parameters of coal in Indian coal basins. *Energy Sources* **4**(4):

PETERS, K.E. & MOLDOWAN,J.M. 1993 Guidelines to interpretation. In: *The Biomarker Guide: Interpreting molecular fossils in petroleum and ancient sediments*. Peters & Moldowan Eds. Prentice Hall, p. 110-265.

PÜTTMANN, W.; WOLF, M. & WOLFF-FISCHER, E. 1986 Chemical characteristics of Liptinite macerals in humic and sapropelic coals. *Advances in Organic Geochemistry*, 1985. **10**:625-632.

SCHNEIDER,R.L.; MUHLMANN,H.; TOMMASI,E.; MEDEIROS,R.S.; DAEMON, R.F. & NOGUEIRA, A.A. 1974 Revisão estratigráfica da Bacia do Paraná. In: Congresso Brasileiro de Geologia, 28. *Anais*, Porto Alegre, SBG, **1**:41-66

SCHOPF, J.M. 1960 Sampling of coal beds. Contributions to General Geology. *Geological Survey Bulletin*. Washington, U.S.Gov.Printing Office, 1111B.

SEIFERT, W.K. & MOLDOWAN, J.M. 1986 Use of biological markers in petroleum exploration. In: Biological markers in the sedimentary record. R.B. Johns Ed. *Methods in Geochemistry and Geophysics*. p. 261-290, Elsevier.

SOUZA LIMA, L.M.F. 1984 *Contribuição ao estudo petrográfico e geoquímico de carvões da Jazida de Chico Lomã, Santo Antonio da Patrulha, RS*. Master Thesis. PPGEEMM, UFRGS, Porto Alegre, 175 p. Unpublished.

STACH, E.; MACKOWSKY, M. Th.; TEICHMULLER, M.; TAYLOR, G. H.; CHANDRA, D. & TEICHMULLER, R. 1982 *Textbook of coal petrology*, Gebrüder Borntraeger Berlin-Stuttgart, 535 p.

TEN HAVEN, H.L.; LITTKE, R.& RULLKÖTTER, J. 1992 Hydrocarbon biological markers in Carboniferous coals of different maturities. In: Moldowan, J.M.; Albrecht, P. & Philp, R.P. *Biological markers in sediments and petroleum*. Prentice Hall, New Jersey. p. 142-155.

TISSOT, B.P. & WELTE, D.H. 1978 *Petroleum Formation and Occurrence*. Springer Verlag, Berlin, 538 pp.