

Table OA12. Elemental data of hydrous pyrolysis samples.

Sample #	Formation	Nitrogen (wt.%)	Carbon (wt.%)	Hydrogen (wt.%)	Oxygen (wt.%)	total Sulfur (wt.%)	total Iron (wt.%)	Total (wt.%)	org. Sulfur (wt.%)	H/C	O/C	N/C	org S/C	orgS/ (orgS+C)
31	Shublik	1.31	54.38	6.05	4.20	15.00	10.20	91.14	3.29	1.33	0.058	0.266	0.0226	0.0221
33	Hue	1.41	53.97	5.3	5.80	16.87	15.30	98.65	*	1.17	0.081	0.208	*	*
34	Hue	1.16	63.85	5.02	3.49	13.81	11.10	98.43	1.06	0.94	0.041	0.284	0.0062	0.0062
35	Hue	0.92	58.54	4.67	3.51	17.00	15.80	100.44	*	0.95	0.045	0.224	*	*
38	Hue	1.97	71.27	7.43	9.28	5.93	1.18	97.06	4.57	1.24	0.098	0.181	0.0240	0.0235
42	Hue	1.96	68.74	6.05	17.49	3.68	0.18	98.10	3.47	1.05	0.191	0.096	0.0189	0.0186

Organic Sulfur = total S wt% - ((Fe wt%/0.46547) - Fe wt%)

* = all sulfur is accommodated by Iron Sulfides

H/C = (H wt%/1.00794)/(C wt%/12.011)

O/C = (O wt%/15.9994)/(C wt%/12.011)

N/C = (N wt %/14.0674)/(C wt%/12.011)

orgS/C = (orgS wt%/32.066)/(C wt%/12.011)

orgS/orgS+C = (orgS wt%/32.066)/((orgS wt %/32.066)+(C wt%/12.011))