

APPENDIX 6

Stable isotope composition, molecular and molecular indices of gases generated from coals and shales by hydrous pyrolysis experiments at 330 and 360°C for 72 h

Sample code	HP temp. [°C]	Stable isotopes [‰]											Gas indices						Isotopic indices				
		C a r b o n								H y d r o g e n			Nitrogen										
		$\delta^{13}\text{C}$ (CH ₄)	$\delta^{13}\text{C}$ (C ₂ H ₆)	$\delta^{13}\text{C}$ (C ₃ H ₈)	$\delta^{13}\text{C}$ (i-C ₄)	$\delta^{13}\text{C}$ (n-C ₄)	$\delta^{13}\text{C}$ (i-C ₅)	$\delta^{13}\text{C}$ (n-C ₅)	$\delta^{13}\text{C}$ (CO ₂)	$\delta^2\text{H}$ (CH ₄)	$\delta^2\text{H}$ (C ₂ H ₆)	$\delta^2\text{H}$ (C ₃ H ₈)	$\delta^{15}\text{N}$ (N ₂)	C _{HC}	C ₂ /C ₃	C ₃ /(n-C ₄ + i-C ₄)	C ₃ /C ₄₊	i-C ₄ / n-C ₄	CDMI	$\Delta^{13}\text{C}$ (C ₂ -C ₁)	$\Delta^{13}\text{C}$ (C ₃ -C ₂)	$\Delta^2\text{H}$ (C ₂ -C ₁)	$\Delta^2\text{H}$ (C ₃ -C ₂)
Upper Silesian Coal Basin																							
Br-20st	330	-34.8	-28.7	-26.5	-26.9	-26.5	-25.4	-27.3	-12.2	-327	-271	-242	-2.1	4.59	1.78	2.15	0.56	0.41	86.1	6.1	2.3	56	28
	360	-35.3	-27.9	-28.1	-27.1	-26.2	-25.2	-26.1	-13.2	-315	-268	-239	1.7	4.63	1.69	2.05	0.74	0.61	71.1	7.4	-0.2	47	29
Br-20c	330	-35.7	-27.8	-26.4	-26.0	-25.4	-25.0	-24.8	-21.6	-270	-219	-182	-0.3	4.91	2.05	2.34	0.37	0.50	29.4	7.9	1.4	51	37
	360	-35.5	-26.1	-24.9	-25.9	-24.1	-27.5	-24.4	-21.6	-294	-225	-178	-0.5	6.07	2.43	2.69	2.00	0.50	17.1	9.4	1.3	69	47
Br-23c	330	-35.3	-27.8	-26.1	-26.1	-25.6	-24.9	-25.4	-17.0	-285	-247	-227	-0.1	5.08	1.85	1.91	1.19	0.45	39.3	7.5	1.7	38	20
	360	-36.4	-26.5	-25.6	-26.2	-24.7	-24.6	-24.8	-17.8	-302	-250	-228	-0.2	4.84	2.10	26.85	1.57	0.45	32.2	9.8	1.0	52	22
Br-23sb	330	-37.1	-29.2	-28.0	-25.9	-26.4	-26.3	-26.7	-17.2	-305	-244	-242	-0.4	4.53	1.79	1.45	0.35	0.61	59.6	7.8	1.2	61	2
	360	-37.1	-27.5	-27.4	-26.6	-25.2	-25.3	-25.5	-18.3	-310	-244	-239	0.2	4.95	2.01	1.54	0.52	0.55	50.6	9.6	0.1	66	6
MI-21c	330	-37.5	-27.9	-26.6	-26.4	-25.7	-50.6	-25.1	-20.6	-293	-252	-223	-0.7	4.71	2.07	2.10	1.35	0.62	36.0	9.6	1.3	42	29
	360	-36.2	-26.5	-25.5	-26.1	-24.7	-25.4	-24.7	-21.1	-292	-237	-207	-0.6	5.25	2.29	2.40	0.77	0.52	26.8	9.7	1.0	55	29
MI-21sb	330	-36.3	-29.4	-28.0	-26.1	-26.3	-25.5	-25.8	-22.6	-316	-258	-243	n.a.	4.11	1.88	1.36	0.48	1.03	42.6	7.0	1.4	58	15
	360	-37.0	-28.7	-27.0	-26.6	-26.8	-25.1	-26.1	-23.2	-310	-250	-236	-1.0	4.98	2.27	1.66	0.70	0.80	32.1	8.4	1.6	60	14
Si-22st	330	-39.2	-31.4	-30.4	-29.7	-29.3	-28.3	-29.4	3.1	-310	-248	-217	-5.6	3.32	1.60	1.26	0.41	0.55	98.3	7.7	1.0	62	31
	360	-38.7	-30.7	-30.8	-30.6	-30.1	-30.8	-29.9	3.7	-307	-255	-218	-1.5	3.69	1.67	1.30	0.50	0.57	96.4	8.0	-0.1	52	37
Si-22c	330	-37.3	-28.3	-26.8	-27.0	-25.7	-25.6	-25.7	-18.7	-298	-256	-231	-2.1	3.76	1.78	2.28	1.07	0.52	54.2	8.9	1.5	42	25
	360	-37.2	-27.1	-25.7	-25.6	-24.5	-26.2	-25.2	-20.2	-290	-229	-188	-0.9	4.60	2.10	2.64	1.98	0.53	29.1	10.1	1.4	61	41
Si-23st	330	-36.3	-28.6	-27.4	-26.8	-27.7	-26.6	-26.0	2.8	-318	-261	-233	-5.6	2.99	1.57	1.51	0.65	0.64	95.0	7.7	1.2	57	28
	360	-37.1	-27.8	-27.0	-27.0	-27.9	-27.5	-26.6	3.2	-316	-264	-229	-4.3	3.84	1.73	1.51	0.69	0.64	93.8	9.3	0.8	53	34
Si-23c	330	-37.9	-27.4	-26.1	-25.3	-24.6	-24.3	-25.7	-18.9	-304	-250	-224	-3.4	4.00	1.87	2.32	1.41	0.55	58.5	10.5	1.3	54	26
	360	-37.0	-27.1	-26.1	-26.9	-25.4	-25.8	-25.2	-19.5	-303	-246	-207	-1.3	4.57	2.03	2.49	1.68	0.55	42.9	9.9	0.9	57	39
Lublin Coal Basin																							
Bo-20c	330	-37.4	-28.4	-26.5	-26.9	-26.4	-25.7	-25.7	-21.8	-313	-261	-238	0.9	3.59	1.77	2.08	1.32	0.49	53.8	9.0	1.8	52	23
	360	-37.4	-27.4	-26.6	-27.1	-25.4	-24.4	n.a.	-21.7	-308	-252	-219	0.1	4.25	1.93	2.27	1.55	0.48	35.9	10.1	0.8	56	33
Bo-20sb	330	-35.5	-28.2	-26.5	-28.3	-28.1	-26.1	-26.3	-20.6	-323	-270	-251	-0.5	3.56	1.84	1.84	0.60	0.31	66.9	7.3	1.7	53	19
	360	-35.5	-27.1	-26.6	-27.2	-25.5	-26.8	-24.9	-20.5	-313	-260	-244	-0.6	4.02	1.71	1.63	0.62	0.31	54.4	8.4	0.5	53	17

HP temp. – hydrous pyrolysis temperature; C_{HC} = CH₄/(C₂H₆+C₃H₈); C₂/C₃ = C₂H₆/C₃H₈; C₃/C₄₊ = C₃H₈/(i-C₄H₁₀+n-C₄H₁₀+i-C₅H₁₂+n-C₅H₁₂+C₆+C₇); CDMI = (CO₂/[CO₂+CH₄])100 (%); n.a. – not analysed; c – channel coal sample; st – block shale sample collected above top of coal seam; sb – block shale sample collected below bottom of coal seam