Supporting Information

Adsorption of Chloroaromatic Models for Dioxins on Porous Carbons: The Influence of Adsorbate Structure and Surface Functional Groups on Surface Interactions and Adsorption Kinetics

Jon. G. Bell, Xuebo Zhao, Yaprak Uygur and K. Mark Thomas*

Northern Carbon Research Laboratories, Joseph Swan Institute for Energy Research, School of Chemical Engineering and Advanced Materials, Bedson Building, Newcastle University, Newcastle upon Tyne, NE1 7RU, U.K.

(* Authors to whom all correspondence should be addressed: E-mail: mark.thomas@ncl.ac.uk)

Contact: Professor K. Mark Thomas

E-mail: mark.thomas@ncl.ac.uk

Tel: +44 191 222 6839

Fax: +44 191 222 6929

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Table S1: Pore volumes and surface areas of carbons used in the study of the effect of porous structure

Carbon	Total Pore Volume / $cm^3\ g^{-1}$	Micropore Volume / $cm^3\ g^{-1}$ (< 2 nm)	Micropore Volume / $cm^3\ g^{-1}$ (< 0·7 nm)	Surface Area $m^2\ g^{-1}$
Adsorptive	N_2, 77 K,	N_2, 77 K, DR†	CO_2, 273 K, DR†	N_2, 77 K BET
G209	0.494	0.475	0.188	978
BAX950*	0.905	0.438	0.152	1238
BK	0.185	0.122	0.119	308

† Linear part of D-R graph was used in micropore volume calculation. * Particle size fraction 1.18 - 1.7 mm .Total pore volumes were calculated extrapolating the isotherm data to $p/p^0 = 1$ using densities of 0.8081 g cm^{-3} and 1.032 g cm^{-3} for nitrogen and carbon dioxide, respectively

Table S2. Parameters for fitting the Langmuir-Freundlich isotherm to the adsorption isotherms of chloroaromatic species

Adsorptive	Temperature	K	q	Amount Adsorbed Range /mmol g^{-1}
Chlorobenzene/G209				
	353.11 ± 0.05	8.99	0.40	0 – 2.22
	372.36 ± 0.16	4.64	0.40	0 – 2.17
	393.65 ± 0.07	1.17	0.40	0.47 – 2.10
	423.43 ± 0.10	0.27	0.41	0.44 – 2.12
	452.62 ± 0.09	0.10	0.44	0.48 – 2.02
1,3 dichlorobenzene /G209				
	348.93 ± 0.09	269.55	1.24	0 – 2.05
	372.96 ± 0.08	101.50	0.61	0 – 2.04
	393.23 ± 0.07	40.68	0.56	0 – 2.01
	422.73 ± 0.17	7.06	0.52	0.63 – 2.06
	452.62 ± 0.11	1.51	0.49	0.54 – 2.09
2-chloroanisole /G209				
	407.81 ± 0.24	81.86	0.85	0.54 – 1.54
	423.40 ± 0.14	32.34	0.63	0.50 – 1.68
	452.97 ± 0.10	4.22	0.53	0.54 – 1.51
2-chlorotoluene /G209				
	353.42 ± 0.06	415.24	1.22	0 – 1.67
	372.66 ± 0.09	76.48	0.55	0 – 1.86
	392.68 ± 0.08	7.11	0.41	0.60 – 2.33
	422.77 ± 0.09	2.03	0.44	0.49 – 2.33
	452.98 ± 0.10	0.65	0.44	0.50 – 2.35
2-chlorotoluene/ GOX24				

	352.79 ± 0.07	123.47	0.82	0.48 – 1.36
	373.30 ± 0.09	33.14	0.66	0.38 – 1.35
	393.31 ± 0.11	5.62	0.52	0.39 – 1.32
	423.09 ± 0.08	0.57	0.47	0.45 – 1.38
	452.67 ± 0.08	0.16	0.53	0.47 – 1.33
2-chlorotoluene/ GH_2				
	352.77 ± 0.07	171.14	0.54	0 – 2.49
	373.29 ± 0.08	68.26	0.53	0 – 2.07
	392.67 ± 0.05	6.45	0.36	0.69 – 2.09
	422.77 ± 0.08	4.61	0.48	0.51 – 2.00
	452.97 ± 0.09	0.94	0.46	0.47 – 2.08

Table S3: Virial parameters A_0 and A_1 values for the adsorption of chlorobenzene, 2-chlorotoluene, 1,3 dichlorobenzene, and 2-chloroanisole on G209 and 2-chlorotoluene on GOX24, and GH_2 in the temperature range 353 K – 453 K

Adsorptive	Carbon	Temperature / K	A_0/ Ln(mol g^{-1} Pa^{-1})	A_1/ ln(mol g^{-1} Pa^{-1})
Chlorobenzene	G209	353.11 ± 0.05	-4.57 ± 0.03	-2057 ± 22
		372.36 ± 0.16	-5.02 ± 0.03	-2289 ± 26
		393.65 ± 0.29	-6.03 ± 0.06	-2453 ± 58
		423.43 ± 0.10	-6.96 ± 0.08	-3333 ± 141
		452.62 ± 0.09	-7.84 ± 0.07	-4615 ± 219
1,3 dichlorobenzene	G209	48.93 ± 0.09	-3.50 ± 0.06	-1404± 115
		372.96 ± 0.08	-4.29 ± 0.04	-1514 ± 28
		393.23 ± 0.25	-4.96 ± 0.01	-1675 ± 8
		422.73 ± 0.17	-6.34 ± 0.03	-1842± 44
		452.62 ± 0.11	-6.92 ± 0.07	-3043 ± 177
2-chloroanisole	G209	407.81 ± 0.24	-5.99 ± 0.07	-1161 ± 84
		423.40 ± 0.14	-6.01 ± 0.04	-1647 ± 52
		452.97 ± 0.10	-7.06 ± 0.06	-2655 ± 174
2-chlorotoluene	G209	353.42 ± 0.06	-3.42 ± 0.15	-1798 ± 84
		372.66 ± 0.09	-4.19 ± 0.06	-2033 ± 44
		392.68 ± 0.08	-4.82 ± 0.07	-2483 ± 74
		422.77 ± 0.09	-5.96 ± 0.05	-3479 ± 138
		452.98 ± 0.10	-6.84 ± 0.02	-4046± 67
2-chlorotoluene	GOX24	352.79 ± 0.07	-5.17 ± 0.08	-1804 ± 81
		373.30 ± 0.09	-6.27 ± 0.06	-1783 ± 103
		393.31 ± 0.11	-6.69 ± 0.01	-2731± 15
		423.09 ± 0.08	-7.59 ± 0.02	-4323 ± 86
		452.67 ± 0.08	-8.48 ± 0.06	-11325± 673
2-chlorotoluene	GH_2	352.77 ± 0.07	-3.39 ± 0.07	-1735 ± 46
		373.29 ± 0.08	-4.23 ± 0.03	-1990 ± 35
		392.67 ± 0.05	-4.74 ± 0.34	-2185 ± 403
		422.77 ± 0.08	-6.39 ± 0.03	-2378 ± 62
		452.97 ± 0.09	-7.30 ± 0.02	-3246 ± 86

Table S4: Virial parameter A_0 and K_H for CO_2 adsorption on G209, GOX24, and GH_2 at 273 K

Carbon	A_0/ ln(mol g^{-1} Pa^{-1})	A_1/ / ln(mol g^{-1} Pa^{-1})	K_H (x 10^{-7}) mol g^{-1} Pa^{-1}
G209	-15.135 ± 0.010	-1083 ± 24	2.672 ± 0.027
GOX24	-15.506 ± 0.017	-536 ± 16	1.844 ± 0.032
GH_2	-14.425 ± 0.037	-1590 ± 73	5.439 ± 0.204

Table S5: Isosteric enthalpies of adsorption of chloroaromatic species and benzene as a function of surface coverage, calculated from Linear interpolation, Langmuir Freundlich (LF) isotherm interpolation, and Virial equation analysis

a) Chlorobenzene adsorption on G209

Amount Adsorbed/ mmol g^{-1}	$Q_{st,n}$ / kJ mol^{-1}			-ΔS/ J K^{-1} mol^{-1}	
	Virial	Linear Interpolation	LF	Linear Interpolation	LF
0	45.06 ± 2.80				
0.1	48.33 ± 2.74				
0.2	51.63 ± 3.18				
0.3	54.92 ± 3.71				
0.4	58.21 ± 4.29				
0.5	61.50 ± 4.90		65.88 ± 3.59		126.15 ± 9.11
0.6			65.31 ± 3.42		129.00 ± 8.68
0.7			64.87 ± 3.29		131.66 ± 8.34
0.8			64.39 ± 3.17		133.78 ± 8.04
0.9		64.13 ± 3.10	63.98 ± 3.04	136.26 ± 7.86	135.80 ± 7.71
1		63.30 ± 3.05	63.58 ± 2.93	137.01 ± 7.74	137.59 ± 7.42
1.1		63.41 ± 2.99	63.17 ± 2.84	139.86 ± 7.59	139.19 ± 7.20
1.2		62.17 ± 2.84	62.81 ± 2.71	139.27 ± 7.21	140.76 ± 6.86
1.3		62.45 ± 2.60	62.44 ± 2.61	142.35 ± 6.59	142.19 ± 6.62
1.4		61.88 ± 2.66	62.10 ± 2.51	143.29 ± 6.74	143.59 ± 6.36
1.5		62.03 ± 7.27	61.74 ±2.41	144.74 ± 18.45	144.90 ± 6.11
1.6		61.26 ± 2.14	61.39 ± 2.32	146.00 ± 5.43	146.14 ± 5.87
1.7		60.72 ± 1.91	61.03 ± 2.22	146.78 ± 4.84	147.33 ± 5.63
1.8		60.21 ± 1.73	60.66 ± 2.13	147.51 ± 4.38	148.46 ± 5.39
1.9		60.48 ± 1.99	60.28 ±2.03	150.19 ± 5.05	149.55 ± 5.15
2		59.43 ± 1.90	59.88 ± 1.94	149.70 ± 4.82	150.57 ± 4.91
2.1		58.77 ± 1.98		149.94 ± 5.02	
2.2		59.15 ± 1.86		152.84 ± 4.71	
2.3		58.28 ± 2.15		152.69 ± 5.46	
2.4		57.96 ± 2.11		153.90 ± 5.36	

b) 2-chloroanisole adsorption on G209

Amount Adsorbed/ mmol g^{-1}	$Q_{st,n}$ / kJ mol^{-1}			-ΔS/ J K^{-1} mol^{-1}	
	Virial	Linear Interpolation	LF	Linear Interpolation	LF
0	38.36 ± 14.32				
0.1	44.23 ± 15.14				
0.2	49.45 ± 15.43				
0.3	54.66 ± 15.72	43.41 ± 14.05		54.89 ± 32.92	
0.4	59.88 ± 16.02	52.71 ± 14.88		79.80 ± 34.87	
0.5	65.10 ± 16.31	60.70 ± 15.07		101.13 ± 35.32	
0.6		66.76 ± 15.04	67.65 ± 14.48	118.07 ± 35.25	120.00 ± 33.93
0.7		71.89 ± 13.43	71.65 ± 13.29	132.71 ± 31.47	132.19 ± 31.13
0.8		75.67 ± 11.97	75.24 ± 12.25	144.11 ± 28.05	143.23 ± 28.70
0.9		78.64 ± 11.97	78.51 ± 11.35	153.54 ± 28.05	153.39 ± 26.58
1		81.34 ± 11.33	81.38 ± 10.54	162.35 ± 26.55	162.50 ± 24.69
1.1		83.88 ± 10.29	83.85 ± 9.78	170.72 ± 24.11	170.66 ± 22.91
1.2		85.98 ± 9.23	86.03 ± 9.21	178.13 ± 21.64	178.16 ± 21.57
1.3		87.18 ± 8.54	87.67 ± 8.78	183.43 ± 20.02	184.42 ± 20.58
1.4		88.30 ± 8.48	89.04 ± 8.71	188.60 ± 19.87	190.19 ± 20.42
1.5		89.25 ± 7.04	89.43 ± 8.97	193.47 ± 16.49	193.82 ± 21.01

Calculated using 408 K, 423 K, and 453 K isotherms

c) 1,3 dichlorobenzene adsorption on G209

Amount Adsorbed/ mmol g^{-1}	$Q_{st,n}$ / kJ mol^{-1}			-ΔS/ J K^{-1} mol^{-1}	
	Virial	Linear Interpolation	LF	Linear Interpolation	LF
0	45.52 ± 3.12				
0.1	47.35 ± 3.06				
0.2	49.18 ± 3.13				
0.3	51.01 ± 3.32				
0.4	52.84 ± 3.61				
0.5	54.67 ± 3.99				
0.6			43.41 ± 10.60		64.15 ± 26.95
0.7			46.11 ± 9.84		73.67 ± 25.03
0.8			48.43 ± 9.14		81.96 ±23.24
0.9		50.06 ± 8.44	50.99 ± 8.24	88.37 ± 21.48	90.62 ± 20.95
1		51.75 ± 7.77	52.75 ± 7.75	94.87 ± 19.77	97.21 ± 19.71
1.1		53.74 ± 7.42	54.40 ± 7.27	101.86 ± 18.88	103.43 ± 18.49
1.2		55.76 ± 6.91	56.01 ± 6.81	108.93 ± 17.57	109.46 ± 17.32
1.3		57.50 ± 6.27	57.54 ± 6.34	115.16 ± 15.95	115.22 ± 16.13
1.4		59.34 ± 5.55	59.03 ± 5.89	121.67 ± 14.11	120.87 ± 14.97
1.5		60.93 ± 5.40	60.49 ± 5.42	127.58 ± 13.73	126.41 ± 13.78
1.6		62.33 ± 4.87	61.93 ± 4.95	133.03 ± 12.40	131.92 ± 12.58
1.7		63.70 ± 4.50	63.38 ± 4.46	138.38 ±11.44	137.44 ± 11.35
1.8		64.56 ± 4.20	64.82 ± 3.96	142.47 ± 10.67	142.99 ± 10.07
1.9		65.79 ± 3.69	66.27 ± 3.40	147.52 ± 9.38	148.61 ± 8.64
2		67.24 ± 3.00	67.77 ± 2.80	153.17 ± 7.63	154.44 ± 7.13
2.1		67.94 ± 2.42		156.92 ± 6.16	
2.2		68.83 ± 2.12		161.26 ± 5.38	
2.3		69.52 ± 1.66		165.23 ± 4.23	
2.4		70.18 ± 1.46		169.16 ± 3.72	

d) 2-chlorotoluene adsorption on G209

Amount Adsorbed/ mmol g^{-1}	$Q_{st,n}$ / kJ mol^{-1}			-ΔS/ J K^{-1} mol^{-1}	
	Virial	Linear Interpolation	LF	Linear Interpolation	LF
0	46.00 ± 1.27				
0.1	49.19 ± 1.54				
0.2	52.37 ± 1.83				
0.3	55.56 ± 2.13				
0.4	58.75 ± 2.44				
0.5	61.94 ± 2.75				
0.6	65.12 ± 3.06		53.23 ± 7.40		90.90 ± 18.77
0.7		56.01 ± 5.98	56.04 ± 6.03	101.26 ± 15.15	101.12 ± 15.29
0.8		58.19 ± 5.14	58.45 ± 4.86	109.54 ± 13.04	110.06 ± 12.32
0.9		60.72 ± 4.16	60.57 ± 3.85	118.60 ± 10.54	117.93 ± 10.07
1		62.53 ± 3.21	62.43 ± 2.98	125.57 ± 8.14	124.33 ± 8.00
1.1		64.49 ± 2.18	64.08 ± 2.30	132.80 ± 5.53	130.19 ± 6.21
1.2		65.59 ± 2.01	65.49 ± 1.85	137.90 ± 5.09	135.62 ± 4.91
1.3		66.14 ±1.68	66.68 ± 1.66	141.75 ± 4.27	140.77 ± 4.15
1.4		66.81 ± 1.51	67.62 ± 1.70	145.56 ± 3.83	145.53 ± 4.10
1.5		67.47 ± 2.03	68.28 ± 1.86	149.43 ±5.14	150.05 ± 4.50
1.6		68.15 ± 2.13	68.46 ± 1.99	153.35 ± 5.41	154.20 ± 5.24
1.7		68.04 ± 2.24		155.33 ± 5.69	
1.8		68.02 ± 2.31		157.68 ± 5.86	
1.9		68.58 ± 2.27		161.21 ± 5.76	
2		68.98 ± 2.88		164.51 ± 7.30	
2.1		69.30 ± 2.99		167.54 ± 7.57	
2.2		68.78 ± 3.08		168.74 ± 7.81	
2.3		68.91 ± 3.35		171.46 ± 8.48	
2.4		68.72 ± 3.26		173.10 ± 8.27	

e) 2-chlorotoluene adsorption on GOX24

Amount Adsorbed/ mmol g^{-1}	$Q_{st,n}$ /kJ mol^{-1}			-ΔS/ J K^{-1} mol^{-1}	
	Virial	Linear Interpolation	LF	Linear Interpolation	LF
0	42.26 ± 2.48				
0.1	53.81 ± 4.86				
0.2		44.30 ± 9.21		93.15 ± 25.66	
0.3		54.51 ± 10.12		115.86 ± 20.65	
0.4		61.17 ± 8.14		133.19 ±17.40	
0.5		66.31 ± 6.86	70.39 ± 6.18	146.53 ±14.91	147.09 ± 15.66
0.6		70.13 ± 5.88	72.33 ± 5.46	155.28 ± 13.74	155.50 ± 13.85
0.7		72.23 ± 5.42	73.96 ± 4.85	162.26 ± 11.58	162.79 ± 12.31
0.8		73.67 ± 4.57	75.34 ± 4.38	170.16 ±11.50	169.19 ± 11.09
0.9		75.70 ± 4.54	76.47 ± 3.98	175.58 ± 9.94	174.83 ± 10.09
1		76.69 ± 3.92	77.39 ± 3.64	178.20 ± 10.14	179.84 ± 9.22
1.1		76.59 ± 4.00	78.05 ± 3.40	182.28 ± 9.28	184.15 ± 8.63
1.2		77.12 ± 3.66	78.50 ± 3.26	186.57 ± 8.80	187.97 ± 8.26
1.3		77.84 ± 3.47	78.52 ± 3.25	188.33 ± 8.03	190.77 ± 8.25
1.4*		77.53 ± 3.17			
1.5*		72.32 ± 0.77			
1.6*		71.98 ± 0.93			
1.7*		72.58 ± 1.20			
1.8*		71.43 ± 0.74			
1.9*		71.74 ± 1.13			
2*		69.64 ± 1.82			
2.1*		69.50 ± 1.94			
2.2*		73.36 ± 0.49			
2.3*		73.42 ± 0.64			

*Calculated using 353 K, 373 K, 393 K, and 423 K isotherm data

f) Adsorption of 2-chlorotoluene on GH_2

Amount Adsorbed/ mmol g^{-1}	$Q_{st,n}$ / kJ mol^{-1}			-ΔS/ J K^{-1} mol^{-1}	
	Virial	Linear Interpolation	LF	Linear Interpolation	LF
0	53.22 ± 3.50				
0.1	55.04 ± 3.50				
0.2	56.85 ± 3.53				
0.3	58.66 ± 3.61				
0.4	60.47 ± 3.72				
0.5	62.28 ± 3.86				
0.6	64.09 ± 4.03	*56.03 ± 8.84		*97.46 ± 22.37	
0.7	65.90 ± 4.23	*59.05 ± 9.32	65.04 ± 6.08	*107.61 ± 23.62	121.68 ± 15.42
0.8		*61.71 ± 6.96	65.78 ± 5.19	*117.12 ± 17.63	126.71 ± 13.16
0.9		*64.50 ± 5.02	66.45 ± 4.38	*126.93 ± 12.72	131.32 ± 11.11
1		66.51 ± 2.74	67.08 ± 3.69	134.48 ± 6.96	135.65 ± 9.36
1.1		66.97 ± 2.56	67.70 ± 3.08	138.25 ±6.50	139.81 ± 7.81
1.2		68.02 ± 2.37	68.30 ± 2.50	143.18 ±6.01	143.83 ± 6.35
1.3		68.85 ± 2.17	68.91 ± 2.05	147.84 ±5.49	147.82 ± 5.20
1.4		69.40 ±1.40	69.50 ± 1.63	151.60 ± 3.55	151.71 ± 4.14
1.5		70.16 ± 1.51	70.10 ± 1.27	155.75 ± 3.83	155.58 ± 3.21
1.6		70.78 ± 0.82	70.70 ± 0.96	159.80 ± 2.07	159.49 ± 2.43
1.7		71.49 ± 0.88	71.33 ± 0.72	164.08 ± 2.24	163.47 ± 1.84
1.8		71.25 ± 0.67	71.96 ± 0.62	166.04 ± 1.70	167.50 ± 1.57
1.9		71.81 ± 0.60	72.65 ± 0.71	169.92 ± 1.53	171.78 ± 1.79
2		72.55 ± 0.95	73.36 ± 1.05	174.34 ± 2.40	176.23 ± 2.66
2.1		73.40 ± 1.34		179.16 ± 3.40	
2.2		72.82 ± 1.61		180.64 ± 4.08	

*Calculated using 373 K, 393 K, 423 K, and 453 K isotherm data

g) Adsorption for benzene adsorption on G209 in the temperature range 298 – 318 K, calculated by linear interpolation between isotherm points

Amount Adsorbed n / mmol g^{-1}	$Q_{st,n}$ / kJ mol^{-1}
0.7	30.37 ± 10.70
0.8	30.53 ± 8.69
0.9	31.85 ± 6.87
1	34.25 ± 5.37
1.1	36.14 ± 4.30
1.2	37.78 ± 3.57
1.3	38.81 ± 2.97
1.4	39.38 ± 3.19
1.5	41.39 ± 1.98
1.6	42.74 ± 1.61
1.7	44.33 ± 1.41
1.8	45.39 ± 1.25
1.9	46.67 ± 1.16
2	47.49 ± 1.12
2.1	48.40 ± 0.97
2.2	49.07 ± 0.76
2.3	49.70 ± 0.74
2.4	50.35 ± 0.63
2.5	50.77 ± 0.64
2.6	51.34 ± 0.64
2.7	52.30 ± 0.67
2.8	52.68 ± 0.42
2.9	52.74 ± 0.46
3	53.27 ± 0.44

Table S6: Comparison of the gradients from graphs of amount adsorbed versus 1/ T at same pressure and relative pressure

Carbon	Pressure /mbar	Gradient (mbar)	Relative Pressure (p/p^0)	Gradient (p/p^0)	Gradient ratio/ (p/p^0)/p
G209					
	0.01	2237 ± 214	1.2×10^{-4}	1067 ± 1.67	0.48
	0.11	2903 ± 141	1.5×10^{-3}	1233 ± 107	0.42
	1.04	2651 ± 23	1.3×10^{-2}	1096 ± 161	0.41
GOX24					
	0.01	1348 ± 172	1.2×10^{-4}	877 ± 103	0.65
	0.11	2476 ± 108	1.5×10^{-3}	1454 ± 122	0.59
	1.04	3036 ± 60	1.3×10^{-2}	1247 ± 108	0.41
GH_2					
	0.01	2288 ± 164	1.2×10^{-4}	1116 ± 91	0.49
	0.11	2759 ± 39	1.5×10^{-3}	1196 ± 40	0.43
	1.04	2343 ± 119	1.3×10^{-2}	874 ± 32	0.37

*Gradient ratio is the gradient of relative pressure divided by gradient from mbar

$$ratio = \left(\frac{dn}{d\left(1/T\right)}\right)_{p/p^0} \Bigg/ \left(\frac{dn}{d\left(1/T\right)}\right)_{p}$$

Table S7: Values of $\ln(k_{n=0})$ for chlorobenzene, 2-chlorotoluene, 1,3 dichlorobenzene, and 2-chloroanisole adsorption on G209 and 2-chlorotoluene adsorption on GOX24 and GH_2

Adsorbate	Carbon	Temperature	$\ln(k_{n=0})$	R^2
Chlorobenzene	G209	353.11 ± 0.05	-7.26 ± 0.18	0.9277
		372.36 ± 0.16	-7.04 ± 0.20	0.9030
		393.65 ± 0.07	-6.77 ± 0.08	0.9807
		423.43 ± 0.10	-6.62 ± 0.08	0.9845
		452.62 ± 0.09	-6.23 ± 0.10	0.9768
2-chlorotoluene	G209	353.42 ± 0.06	-8.47 ± 0.15	0.9773
		372.66 ± 0.09	-7.36 ± 0.14	0.9679
		392.68 ± 0.08	-6.78 ± 0.09	0.9802
		422.77 ± 0.09	-6.29 ± 0.10	0.9623
		452.98 ± 0.10	-5.61 ± 0.12	0.9625
1,3 dichlorobenzene	G209	348.93 ± 0.09	-9.62 ± 0.22	0.9803
		372.96 ± 0.08	-9.22 ± 0.20	0.9793
		393.23 ± 0.07	-8.23 ± 0.15	0.9770
		422.73 ± 0.17	-7.42 ± 0.16	0.9562
mi		452.62 ± 0.11	-6.99 ± 0.09	0.9816
2-chloroanisole	G209	407.81 ± 0.24	-8.36 ± 0.17	0.9577
		423.42 ± 0.14	-7.61 ± 0.09	0.9726
		452.98 ± 0.10	-6.31 ± 0.09	0.9185
2-chlorotoluene	GOX24	352.79 ± 0.07	-7.29 ± 0.10	0.9680
		373.30 ± 0.09	-7.09 ± 0.05	0.9866
		393.31 ± 0.11	-6.64 ± 0.06	0.9914
		423.09 ± 0.08	-6.54 ± 0.08	0.9800
		452.67 ± 0.08	-6.21 ± 0.15	0.9494
2-chlorotoluene	GH_2	352.77 ± 0.07	-8.53 ± 0.13	0.9848
		373.29 ± 0.08	-8.15 ± 0.12	0.9875
		392.67 ± 0.05	-7.56 ± 0.10	0.9832
		422.77 ± 0.08	-7.29 ± 0.06	0.9926
		452.97 ± 0.09	-6.70 ± 0.17	0.9170

Figures

Functional Group Characterization

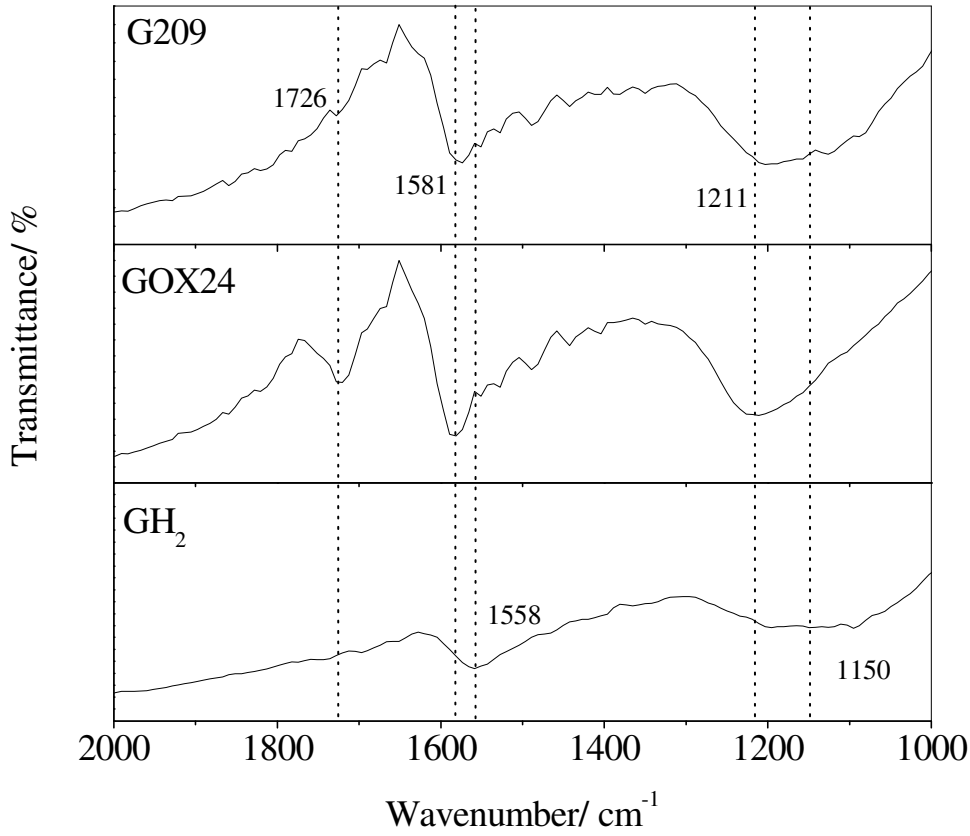

Figure S1: FTIR spectra for G209, GOX24, and GH_2

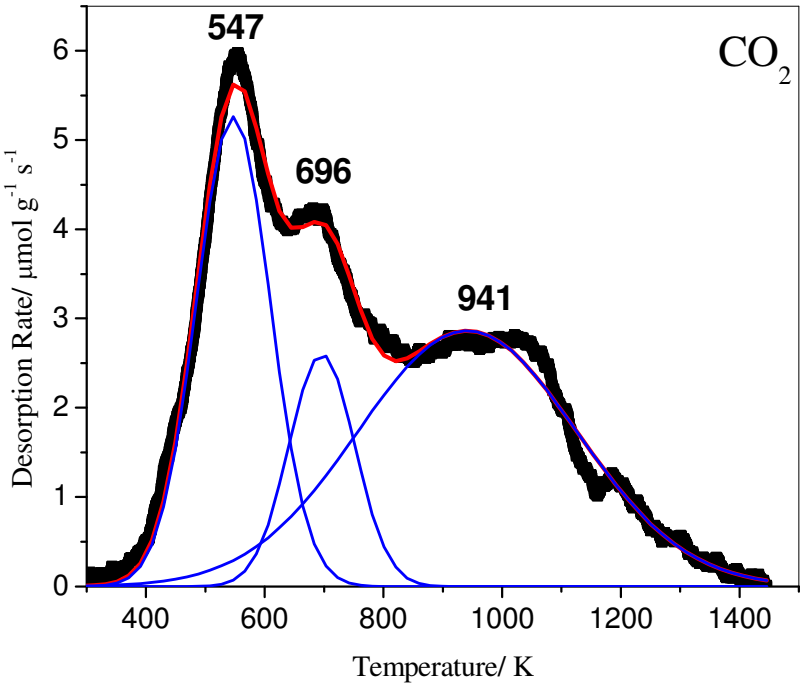

Figure S2a: CO_2 TPD profile for GOX24 showing peak deconvolution : Heating rate 15 K min^{-1}

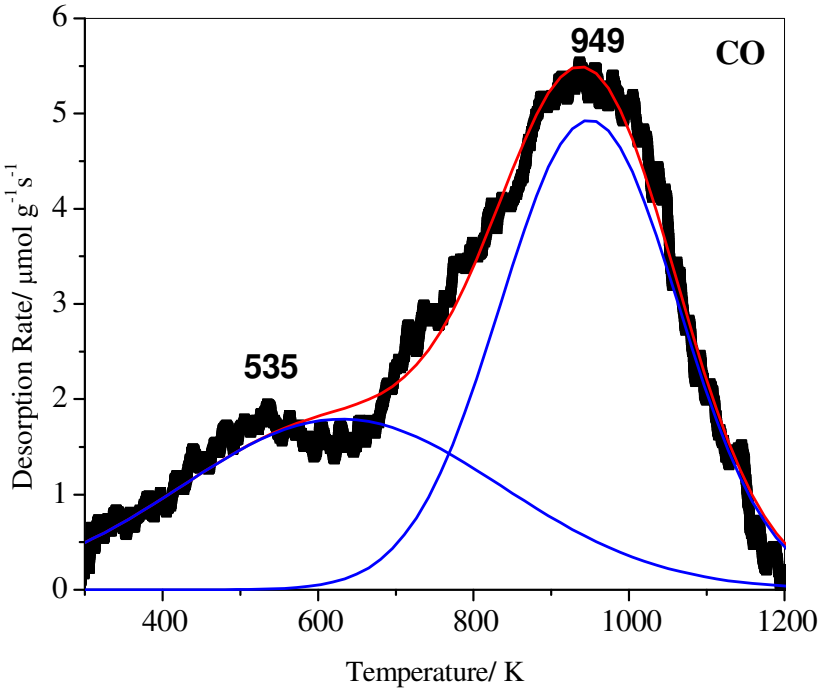

Figure S2 b: CO TPD profile for GOX24 showing peak deconvolution: Heating rate 15 K min^{-1}

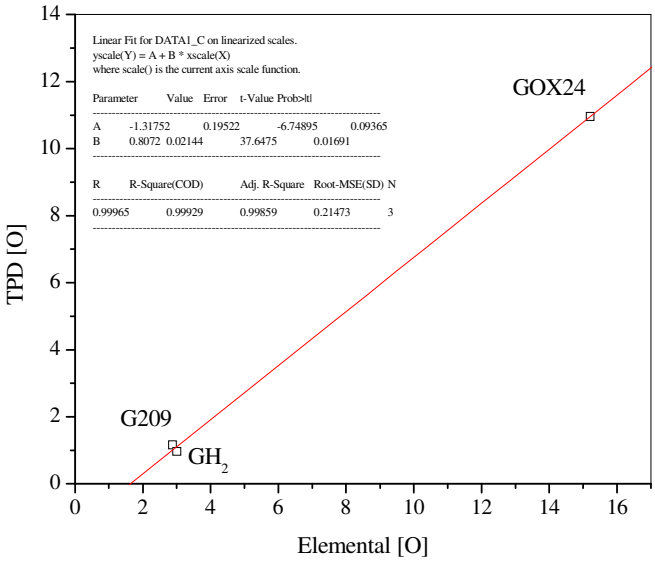

Figure S3: Correlation between chemical analysis and TPD oxygen

Porous Structure Characterization data

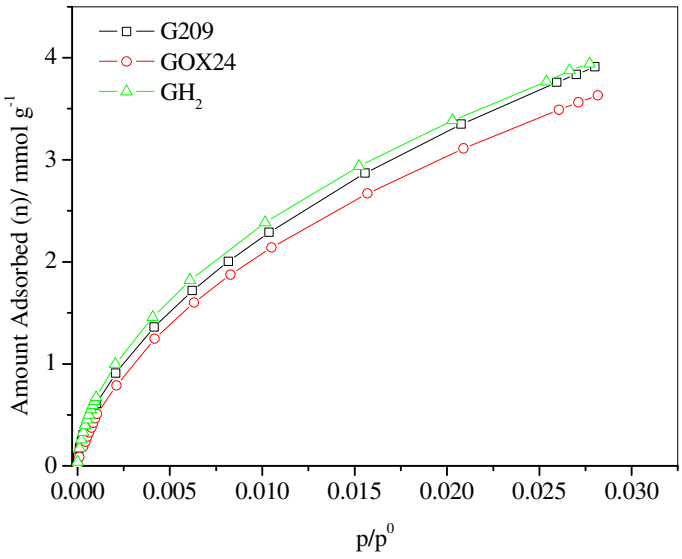

Figure S4 a: CO_2 adsorption isotherms for G209, GOX24, and GH_2 at 273 K

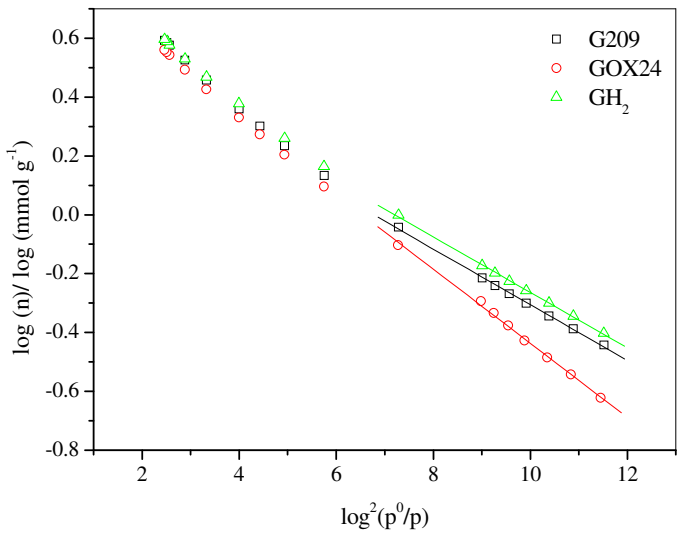

Figure S4 b: Dubinin-Radushkevich graphs for CO_2 adsorption on G209, GOX24, and GH_2; micropore volume corresponds to intercept of linear fit over low relative pressure region (high $\log^2 (p^0/p)$ region

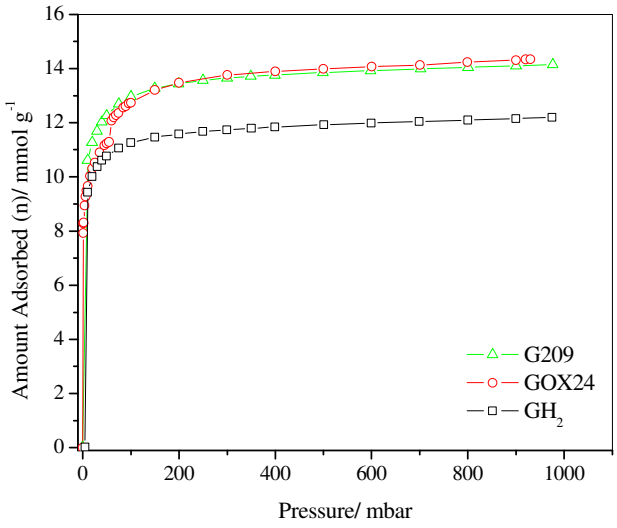

Figure S5a: Isotherms for nitrogen adsorption on G209, GOX24, and GH_2 at 77 K

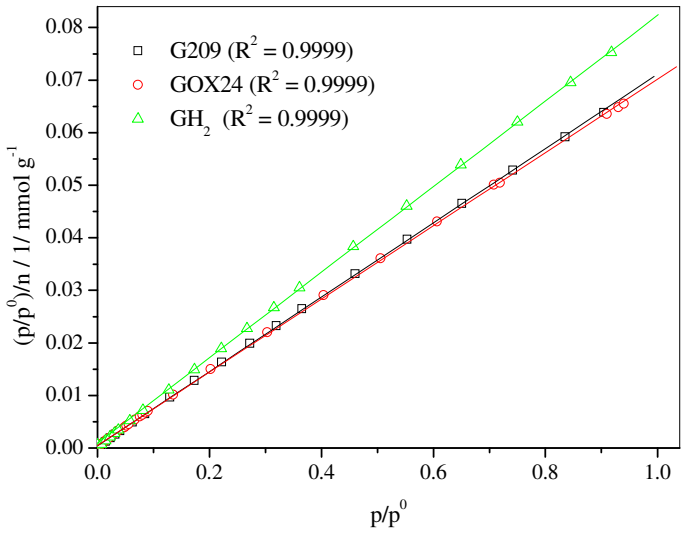

Figure S5b: Langmuir graphs for nitrogen adsorption on G209, GOX24, and GH_2 at 77 K on a p/p^0 basis

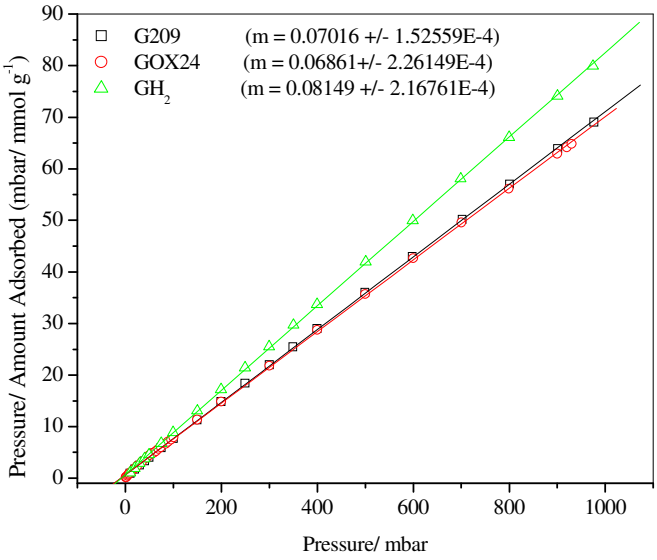

Figure S5c: Langmuir isotherms for nitrogen adsorption on G209, GOX24, and GH_2 at 77 K on a pressure basis

Adsorption of Chloroaromatic species on activated carbons
Isotherms

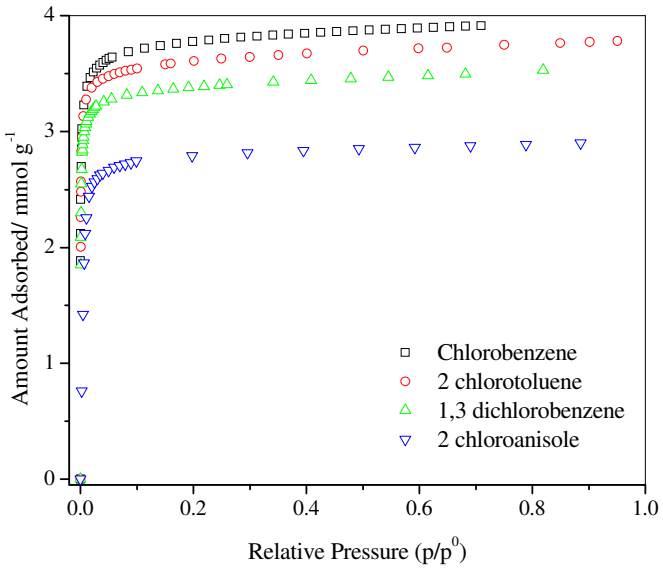

Figure S6: Isotherms for adsorption of chloroaromatic species on chlorobenzene, 2-chlorotoluene, 1,3 dichlorobenzene, and 2-chloroanisole at 313 K

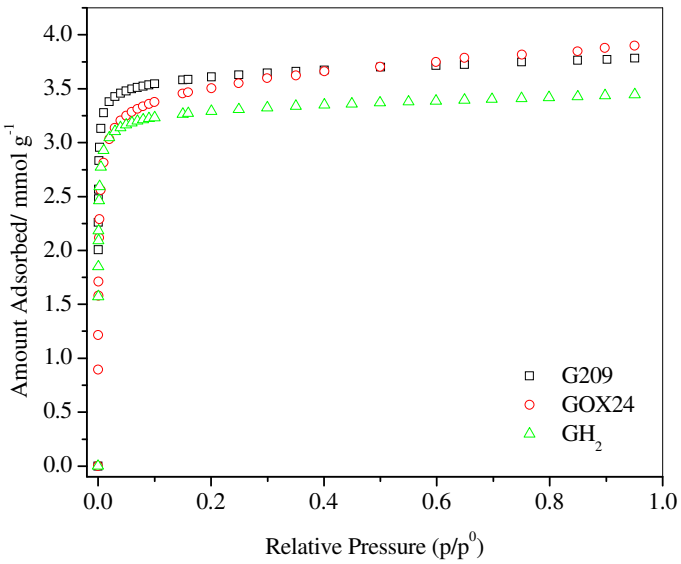

Figure S7: Isotherms for adsorption of 2-chlorotoluene on G209, GOX24, and GH_2 at 313 K

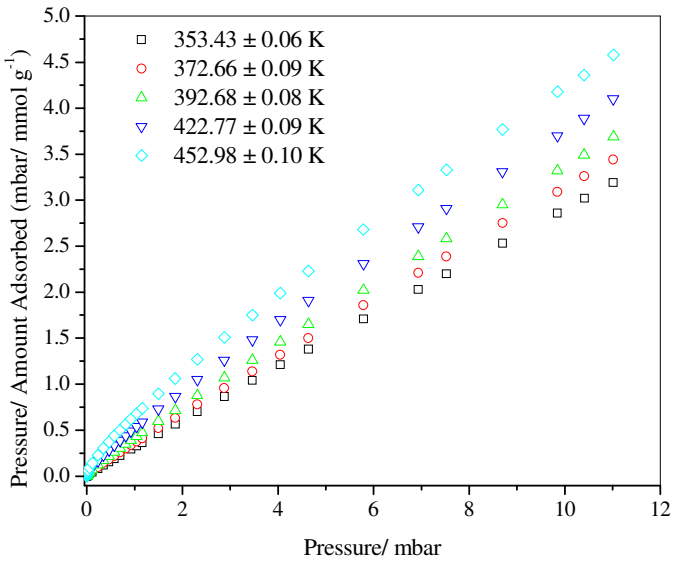

Figure S8a: Langmuir graphs for 2-chlorotoluene on G209 in the temperature range 353 – 453 K

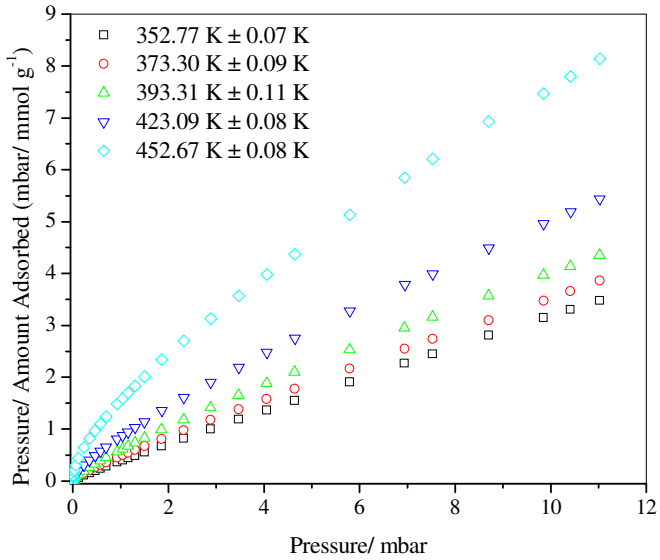

Figure S8b: Langmuir graphs for 2-chlorotoluene on GOX24 in the temperature range 353 – 453 K

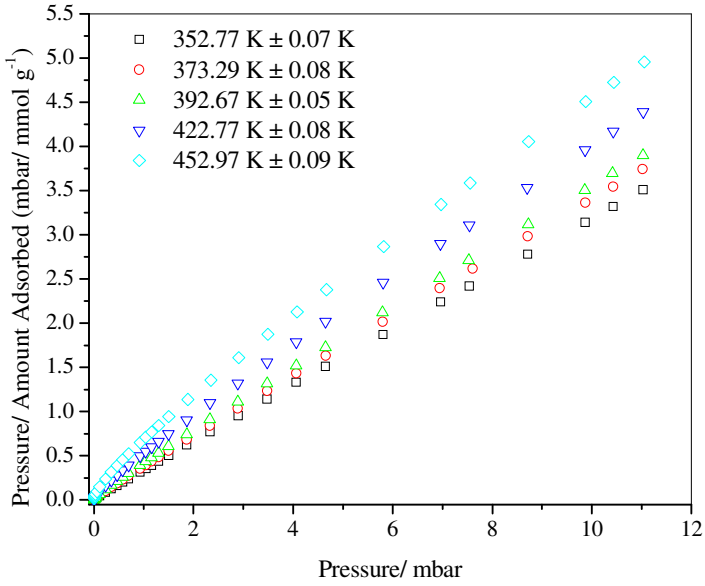

Figure S8c: Langmuir graphs for 2-chlorotoluene on GH_2 in the temperature range 353 – 453 K

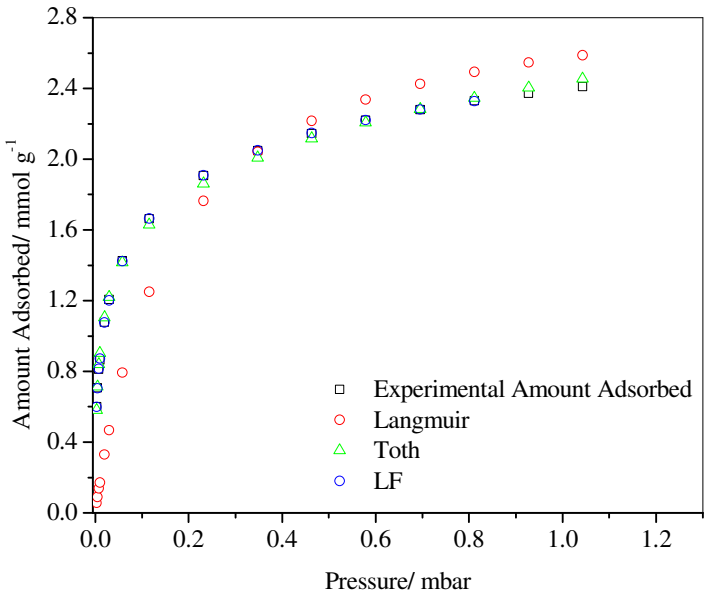

Figure S9 a: Graph of least squares fitting of Langmuir, Toth and LF equations to experimental data for 2-chlorotoluene adsorption on G209 at 393 K

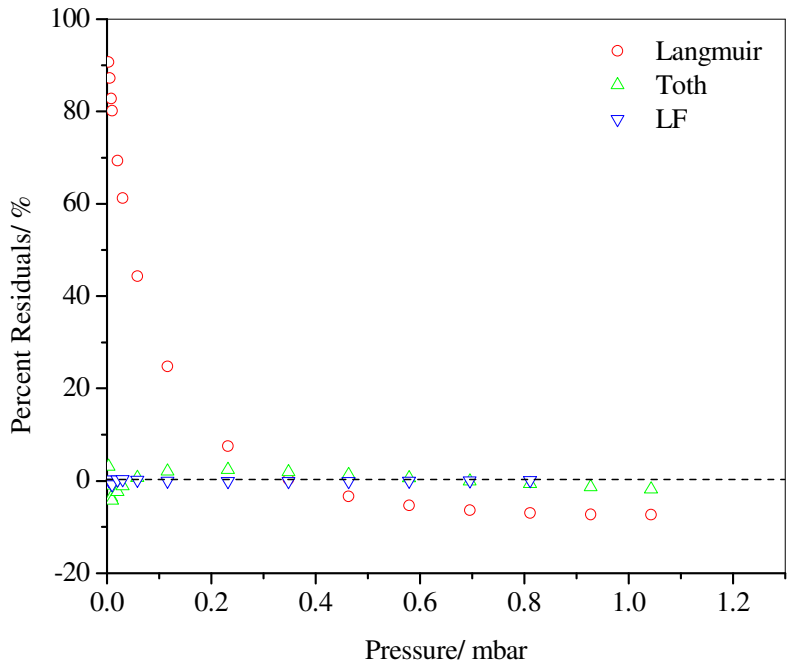

Figure S 9b: Residuals (%) for Langmuir, Toth, and LF equations fits to experimental data for 2-chlorotoluene adsorption on G209 at 393 K

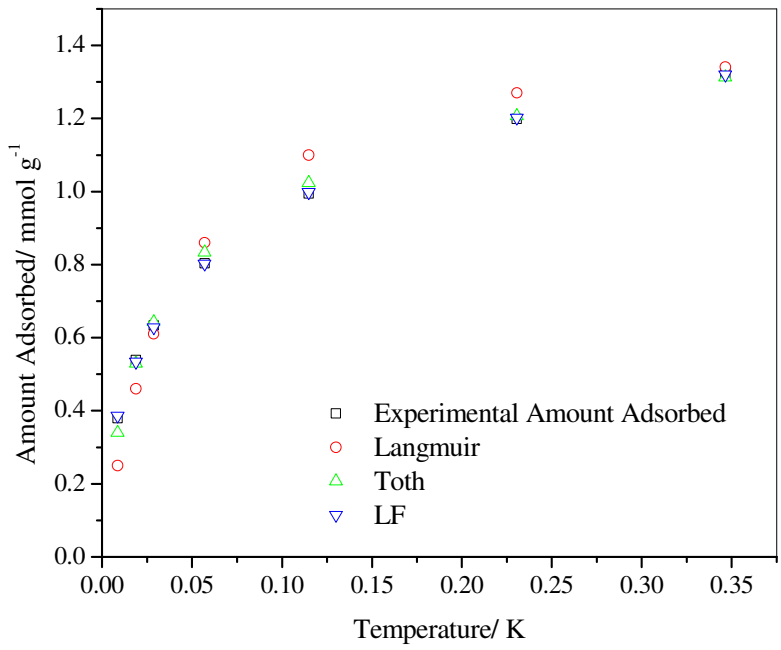

Figure 9c Graph of least squares fitting of Langmuir, Toth, and LF equations to experimental data for 2-chlorotoluene adsorption on GOX24 at 393 K

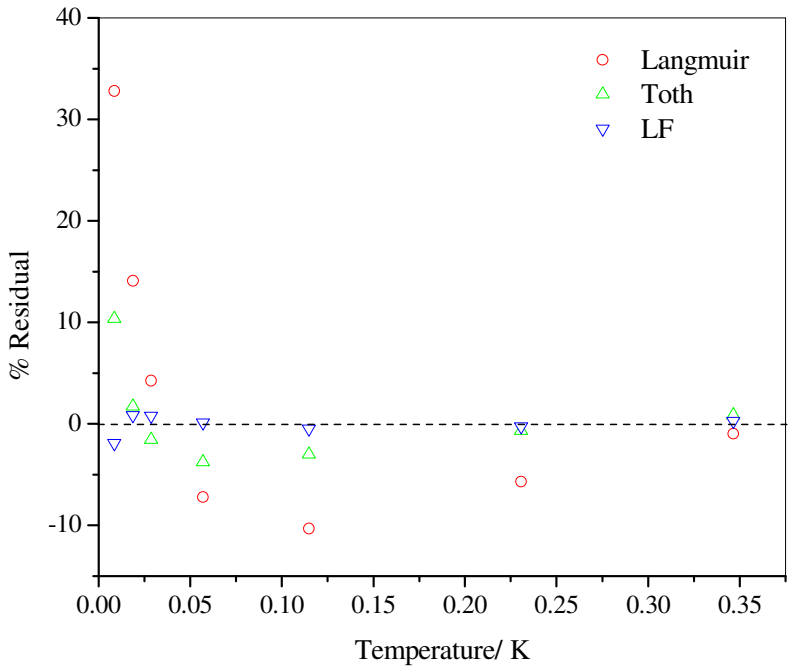

Figure 9d Residuals (%) for Langmuir, Toth, and LF equations fits to experimental data for 2-chlorotoluene adsorption on GOX24 393 K

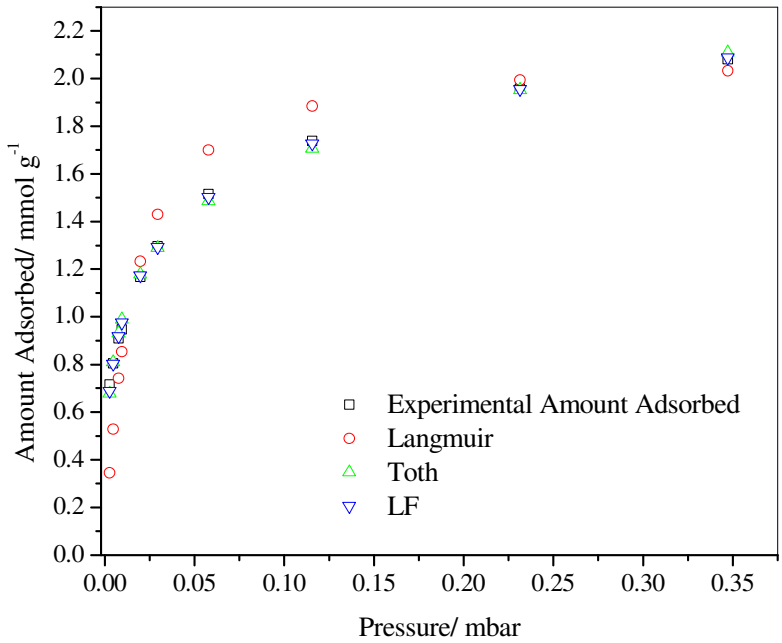

Figure 9e. Graph of least squares fitting of Langmuir, Toth, and LF equations to experimental data for 2-chlorotoluene adsorption on GH2 at 393 K

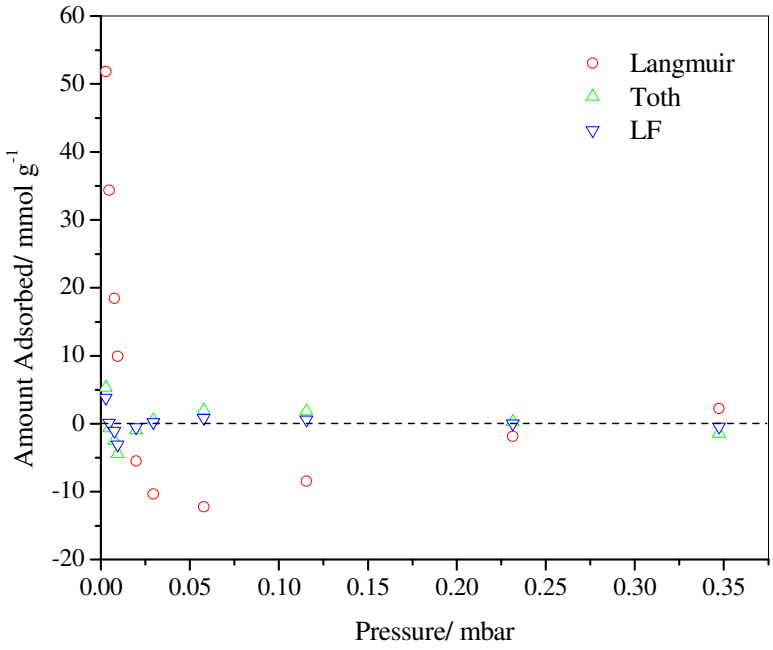

Figure 9f Residuals (%) for Langmuir, Toth, and LF equations fits to experimental data for 2-chlorotoluene adsorption on GH_2 at 393 K

Comparison of Amounts Adsorbed for 2-chlorotoune adsorption in GH_2, G209 and GOX24

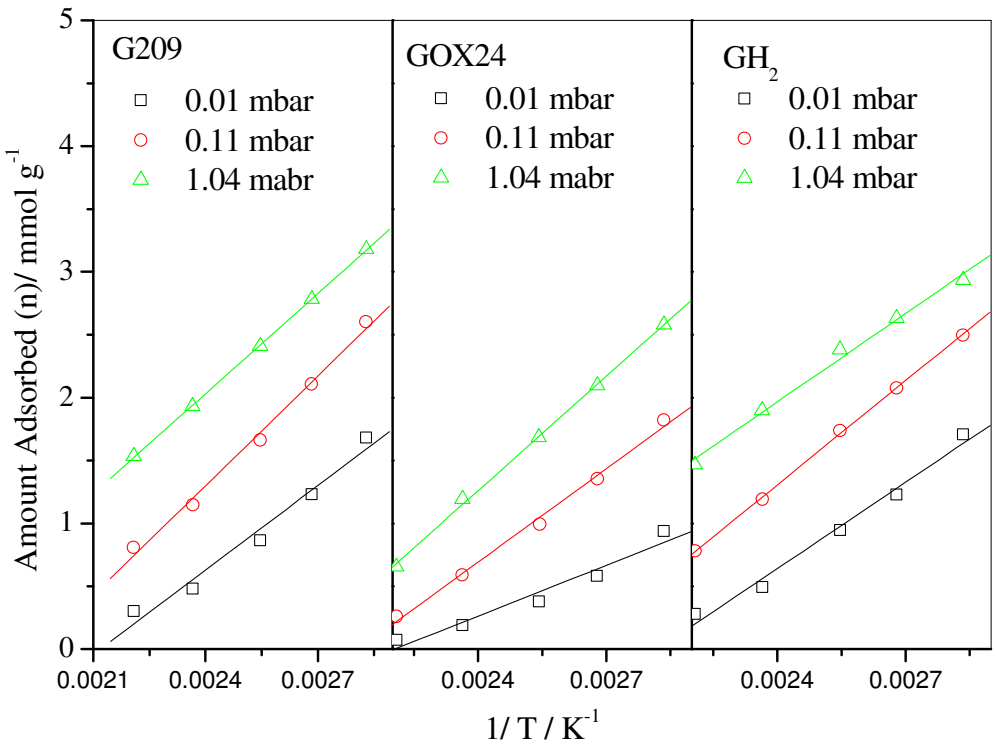

Figure S10 a: The variation of 2-chlorotoluene adsorbed (mmol g^{-1}) vs. 1/ T for G209, GOX24, and GH_2 at 0.01, 0.11, and 1.04 mbar in the temperature range 353 K – 453 K

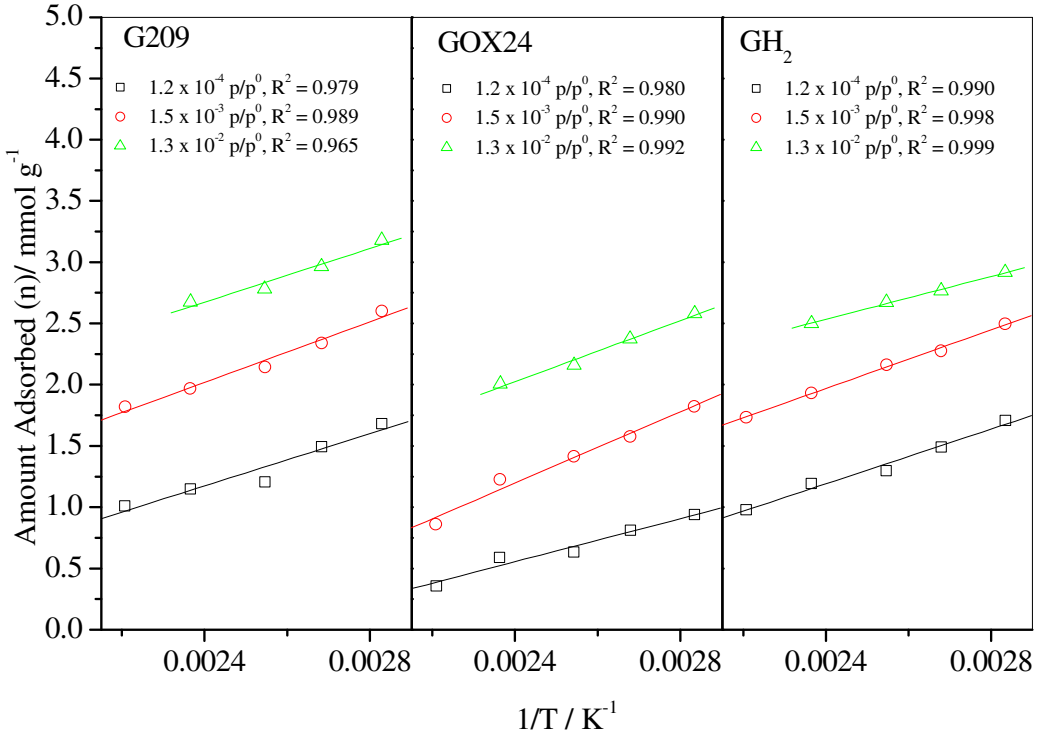

Figure S10 b: The variation of 2-chlorotoluene adsorbed (mmol g^{-1}) vs. 1/ T (1/ K) for G209, GOX24, and GH_2 at 1.2 x 10^{-4}, 1.5 x 10^{-3}, and 1.3 x 10^{-2} p/p^0 in the temperature range 353 K – 453 K

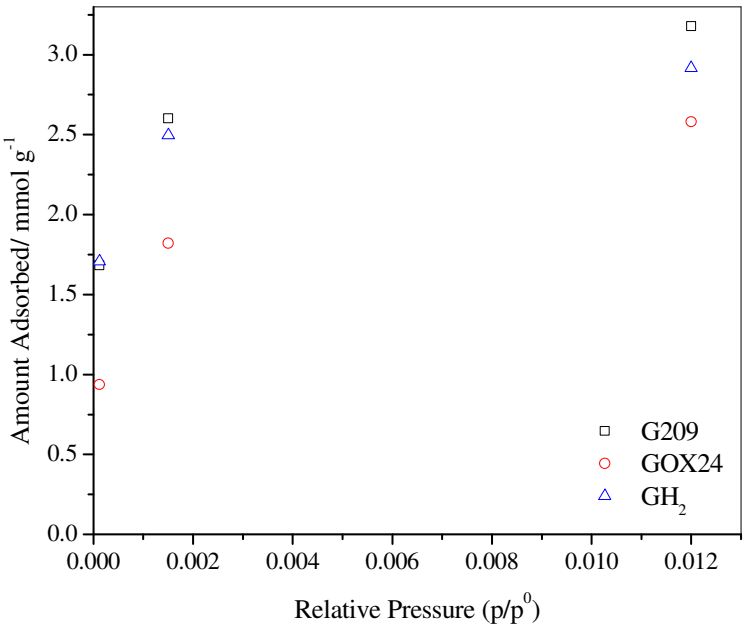

Figure S11 a: Comparison of amounts of 2-chlorotoluene adsorbed on G209,GH_2 and GOX24 at p/p ^{o} at 1.2 x 10^{-4}, 1.5 x 10^{-3} and 1.3 x 10^{-2} p/p ^{o} at 353 K

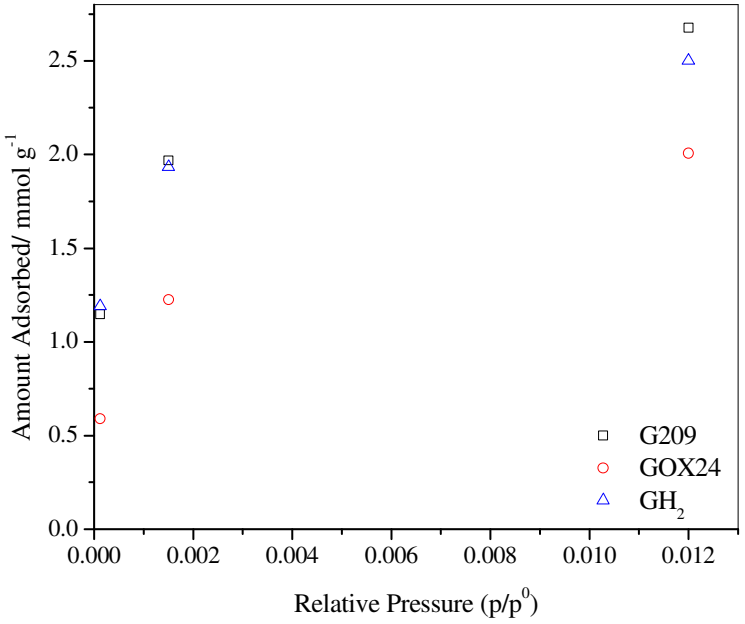

Figure S11 b: Comparison of amounts of 2-chlorotoluene adsorbed on G209,GH_2 and GOX24 at p/p ^{o} at 1.2 x 10^{-4}, 1.5 x 10^{-3} and 1.3 x 10^{-2} p/p ^{o} at 423 K

Adsorption of Benzene on G209

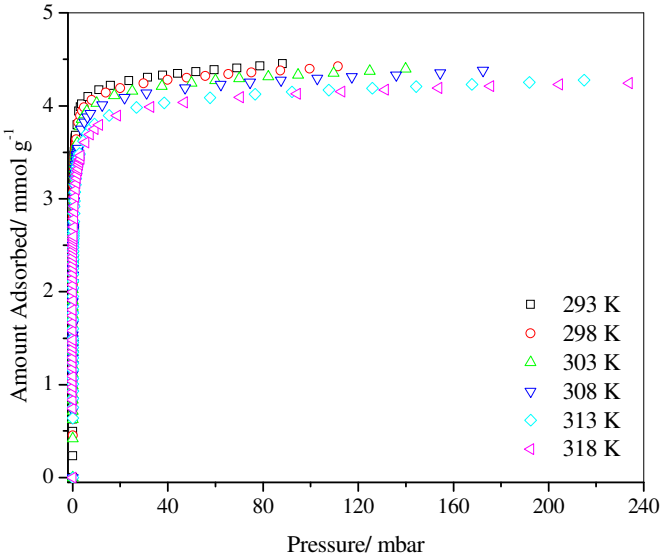

Figure S12a: Isotherms for benzene adsorption on G209 over the temperature range 298-323K

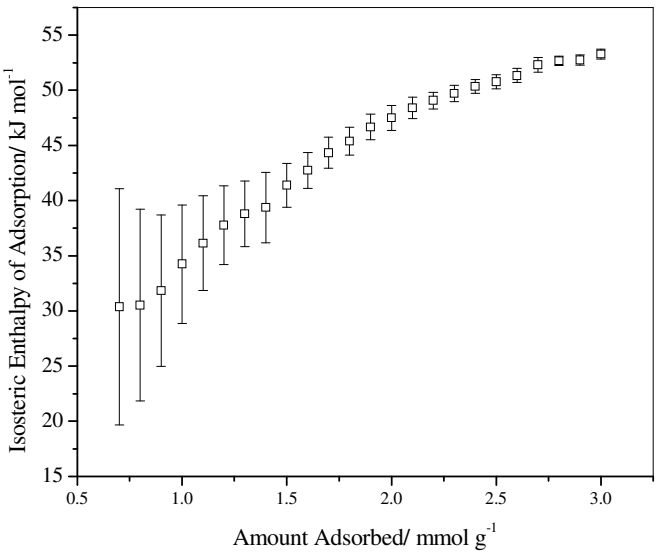

Figure S12b: Isosteric enthalpy vs. amount adsorbed for benzene adsorption on G209 calculated by linear interpolation between adjacent isotherm points

Isotherm Kinetic data

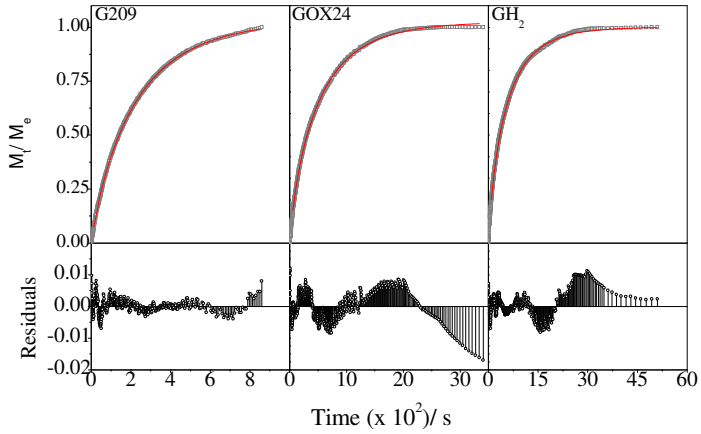

Figure S13: Typical fitting of normalised mass uptake profiles obtained for 2-chlorotoluene adsorption on G209 (p: 0.02983 – 0.05819 mbar), GOX24 (p: 0.00865 – 0.01892 mbar), and GH_2 (p: 0.00514 – 0.00803 mbar) at 353 K using the stretched exponential model and with residuals ≤ 2 %

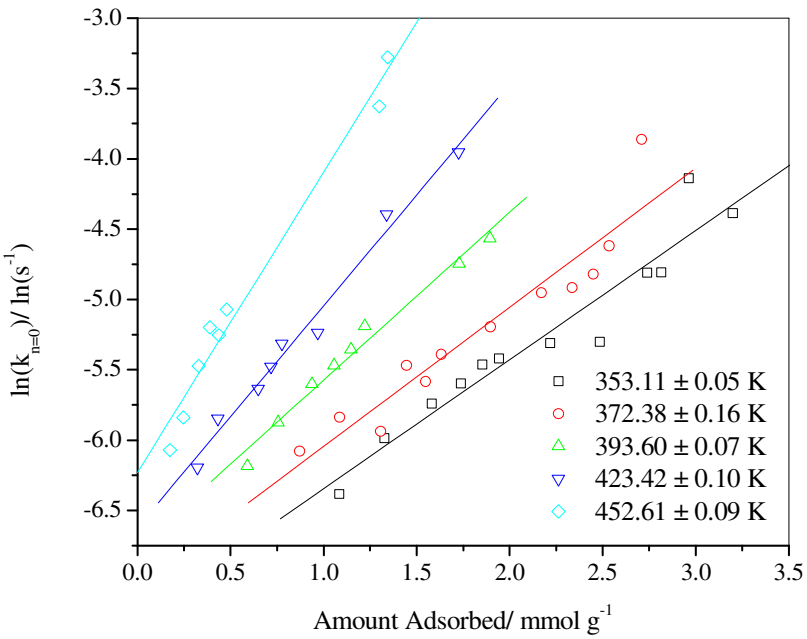

Figure S14a: Graphs of ln(k) versus amount adsorbed for chlorobenzene adsorption on G209 in the temperature range 353 K – 453

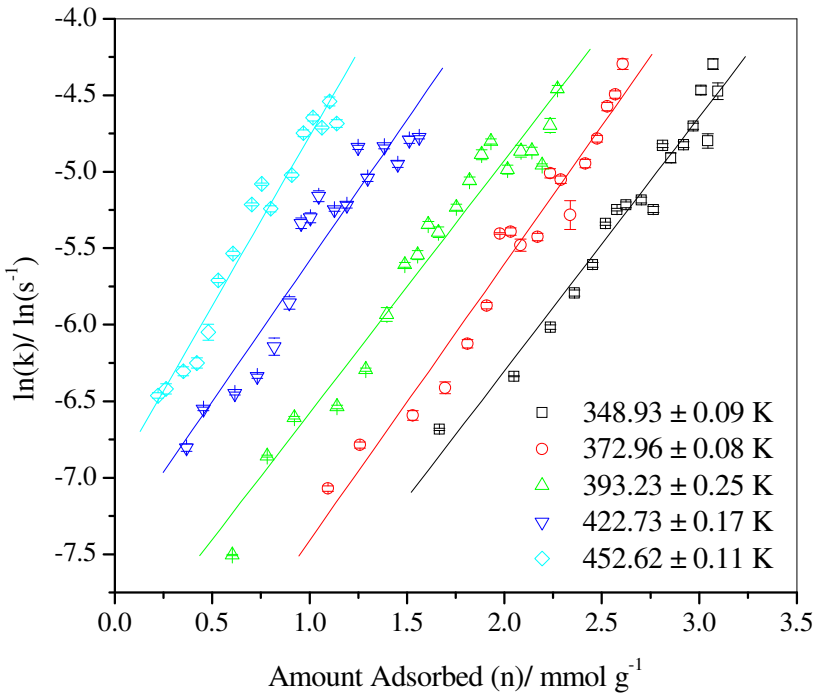

Figure S14b: Graphs of ln(k) versus amount adsorbed for 1,3 dichlorobenzene adsorption on G209 in the temperature range 349 K – 453

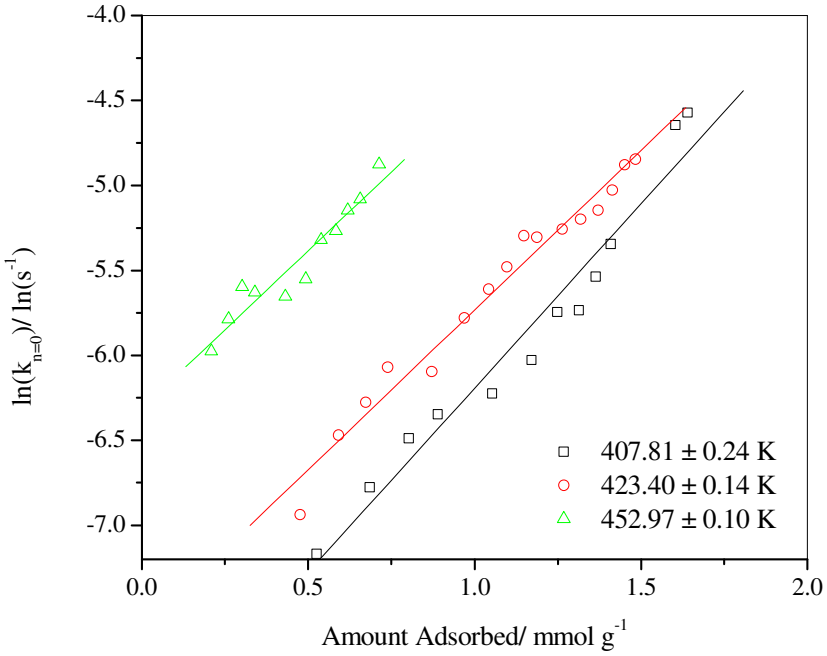

Figure S14c: Graphs of ln(k) versus amount adsorbed for 2, chloroanisole adsorption on G209 in the temperature range 407.8 – 453 K

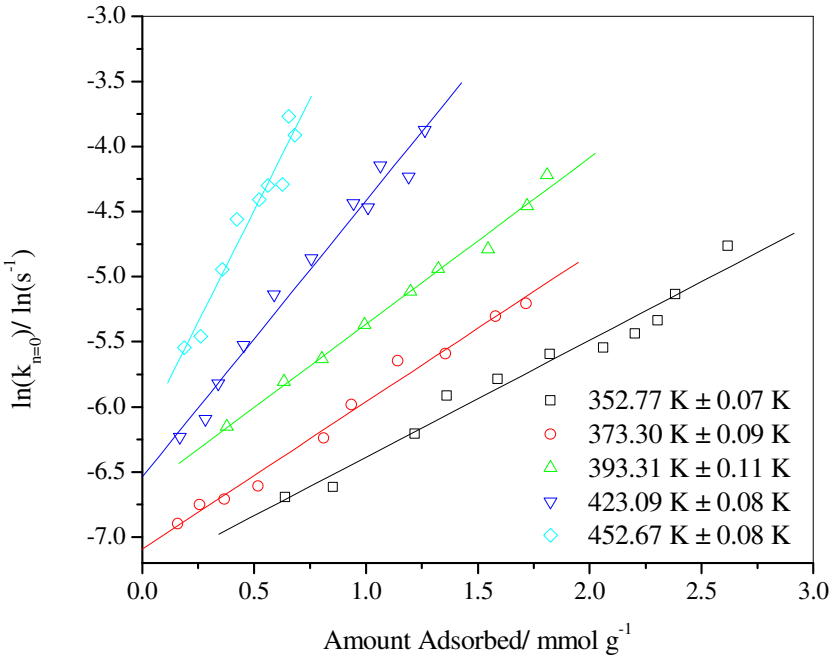

Figure S14d: Graphs of ln(k) versus amount adsorbed for 2, chlorotoluene adsorption on GOX24 in the temperature range 352.8 – 452.7 K

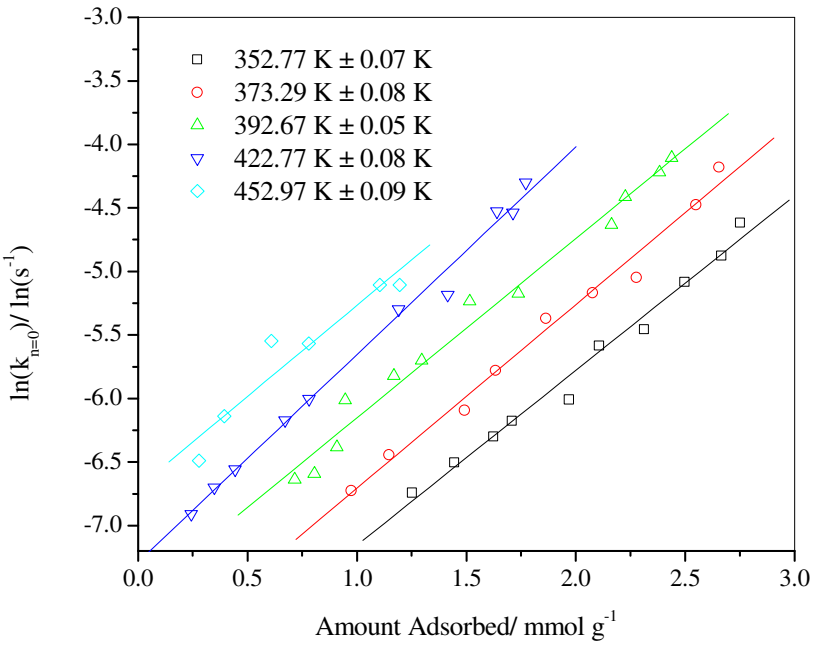

Figure S14e: Graphs of ln(k) versus amount adsorbed for 2, chlorotoluene adsorption on GH_2 in the temperature range 352.8 – 453 K

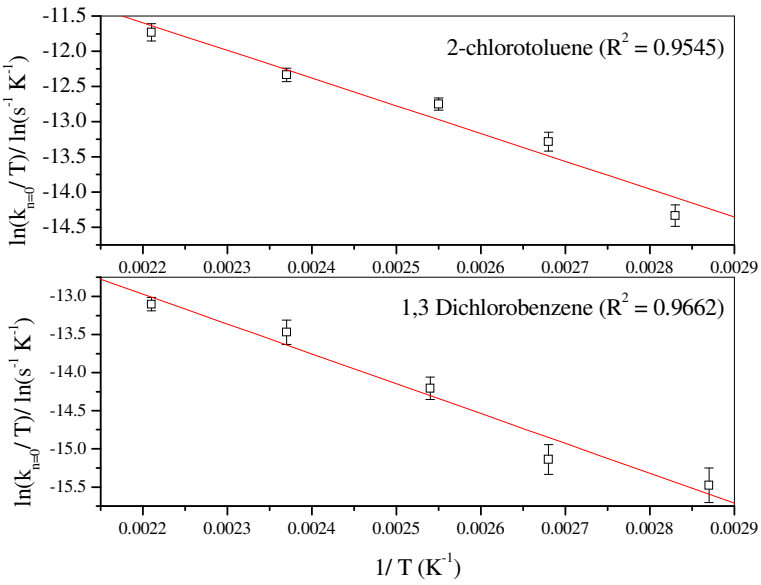

Figure S15:Graph of $\ln(k_{n=0}/T)$ against 1/T for (a) 2-chlorotoluene and (b) 1, 3 dichlorobenzene adsorption on G209 in the temperature range 353 – 453 K