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Supplimentery Informations

Investigations on the development of MCM-41 as a potential mesoporous silica based reference material for the analysis of multi textural properties

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Table 1S Effect of aging on textural properties of glove box samples

Month	Sample code	BET SA, m^2/g	Total PV, cm^3/g	BJH adsorption PD, Å	Wall thickness, (Å)
Freshly Calcined sample (no aging)	SN2(1)	1023	0.936	27.60	17.02
	SN2(2)	1021	0.895	27.54	17.08
	SN2(3)	1026	0.930	27.50	17.12
	SN2(4)	1025	0.986	27.62	17.00
	Mean	1024	0.937	27.56	17.06
	Standard deviation	2.2	0.037	0.055	0.055
(2 months aging)	SN2-GB(1)	979	0.937	27.28	17.46
	SN2-GB(2)	1034	1.030	27.52	17.22
	SN2-GB(3)	1055	1.077	29.42	15.32
	Mean	1023	1.015	28.08	16.66
	Standard deviation	39.2	0.071	1.172	1.172
(4 months aging)	SN2-GB(1)	1036	1.052	27.64	16.64
	SN2-GB(2)	960	0.982	27.54	16.74
	SN2-GB(3)	1101	1.017	27.54	16.74
	Mean	1032	1.017	27.58	16.70
	Standard deviation	70.6	0.035	0.058	0.058
(6 months aging)	SN2-GB(1)	958	0.929	27.50	16.11
	SN2-GB(2)	1015	1.015	27.68	15.93
	SN2-GB(3)	951	0.856	25.52	18.09
	Mean	975	0.934	26.90	16.71
	Standard deviation	35.1	0.079	1.198	1.198
(8 months aging)	SN2-GB(1)	1057	1.015	27.63	17.11
	SN2-GB(2)	987	0.897	27.68	17.06
	SN2-GB(3)	985	0.888	27.47	17.27
	Mean	1009	0.933	27.59	17.15
	Standard deviation	41.0	0.070	0.107	0.107
(10 months aging)	SN2-GB(1)	1118	1.084	27.57	16.29
	SN2-GB(2)	1096	1.036	27.6	16.26
	SN2-GB(3)	1083	1.023	27.59	16.27
	Mean	1099	1.047	27.58	16.28
	Standard deviation	17.7	0.032	0.014	0.014
(12 months aging)	SN2-GB(1)	1061	1.043	27.50	17.25
	SN2-GB(2)	1088	1.04	27.60	17.15
	SN2-GB(3)	1089	1.039	27.41	17.34
	Mean	1079	1.040	27.506	17.25
	Standard deviation	15.9	0.002	0.094	0.094

Table 2S Effect of aging on textural properties of atmospheric condition samples

Month	Sample code	BET SA, m^2/g	Total PV, cm^3/g	BJH adsorption PD, Å	Wall thickness, (Å)
Freshly Calcined sample (no aging)	SN2(1)	1023	0.936	27.60	17.02
	SN2(2)	1021	0.895	27.54	17.08
	SN2(3)	1026	0.930	27.5	17.12
	SN2(4)	1025	0.986	27.62	17.00
	Mean	1024	0.937	27.56	17.06
	Standard deviation	2.2	0.037	0.055	0.055
(2 months aging)	SN2-AC(1)	1002	0.979	27.38	18.38
	SN2-AC(2)	1014	0.967	27.52	18.24
	SN2-AC(3)	1090	1.051	27.38	18.38
	Mean	1035	0.999	27.42	18.34
	Standard deviation	47.7	0.045	0.081	0.081
(4 months aging)	SN2-AC(1)	1032	0.921	27.60	15.84
	SN2-AC(2)	896	0.872	27.60	15.84
	SN2-AC(3)	1003	0.915	27.70	15.74
	Mean	977	0.903	27.64	15.80
	Standard deviation	71.6	0.026	0.058	0.058
(6 months aging)	SN2-AC(1)	1013	0.972	27.60	16.19
	SN2-AC(2)	981	0.903	27.54	16.25
	SN2-AC(3)	987	0.909	27.54	16.25
	Mean	994	0.928	27.56	16.23
	Standard deviation	17.0	0.038	0.035	0.035
(8 months aging)	SN2-AC(1)	1055	0.960	27.52	16.83
	SN2-AC(2)	1028	0.943	27.52	16.83
	SN2-AC(3)	1055	0.910	27.57	16.78
	Mean	1046	0.938	27.540	16.81
	Standard deviation	15.6	0.025	0.032	0.032
(10 months aging)	SN2-AC(1)	983	0.827	27.63	15.85
	SN2-AC(2)	1007	0.851	27.68	15.8
	SN2-AC(3)	1006	0.849	27.64	15.84
	Mean	998	0.842	27.65	15.83
	Standard deviation	13.6	0.013	0.026	0.026
(12 months aging)	SN2-AC(1)	1086	1.030	27.15	16.63
	SN2-AC(2)	1123	1.091	27.25	16.53
	SN2-AC(3)	1037	0.962	27.28	16.5
	Mean	1082	1.027	27.23	16.55
	Standard deviation	43.1	0.064	0.070	0.070

Table 3S PXRD data of glove box samples analyased for one year

Month	Parameter	d_{100}	d_{110}	d_{200}	d_{210}	Std. Dev.	Unit cell $a_{0,}$ (Å)
Freshly Calcined sample (no aging)	2θ Experimental	2.274	3.957	4.54	6.01		44.62
	2θ (d_{100}) Calculated	2.274	2.284	2.27	2.271	0.0065	
	WA 2θ (d_{100})	2.275					
	d Spacing experimental	38.81	22.31	19.43	14.7		
	d Spacing calculated d_{100}	38.81	38.64	38.86	38.89	0.1113	
	WA d_{100}	38.80					
	Intensity (cps)	4460	538	328	120		
(2 months aging)	2θ Experimental	2.286	3.95	4.51	5.897		44.74
	2θ (d_{100}) Calculated	2.286	2.280	2.255	2.229	0.0262	
	WA 2θ (d_{100})	2.281					
	d Spacing experimental	38.62	22.37	19.58	14.97		
	d Spacing calculated d_{100}	38.62	38.75	39.16	39.61	0.4466	
	WA d_{100}	38.70					
	Intensity (cps)	2770	469	302	89		
(4 months aging)	2θ Experimental	2.319	3.988	4.56	6.026		44.28
	2θ (d_{100}) Calculated	2.319	2.302	2.28	2.278	0.0196	
	WA 2θ (d_{100})	2.313					
	d Spacing experimental	38.07	22.14	19.36	14.65		
	d Spacing calculated d_{100}	38.07	38.3476	38.72	38.76	0.3274	
	WA d_{100}	38.16					
	Intensity (cps)	3123	405	269	75		
(6 months aging)	2θ Experimental	2.337	4.026	4.628	6.075		43.61
	2θ (d_{100}) Calculated	2.337	2.324	2.314	2.296	0.0172	
	WA 2θ (d_{100})	2.333					
	d Spacing experimental	37.77	21.93	19.08	14.54		
	d Spacing calculated d_{100}	37.77	37.98	38.16	38.47	0.2956	
	WA d_{100}	37.83					
	Intensity (cps)	3571	452	284	94		
(8 months aging)	2θ Experimental	2.278	3.935	4.529	5.927		44.74
	2θ (d_{100}) Calculated	2.278	2.272	2.264	2.240	0.0165	
	WA 2θ (d_{100})	2.2756					
	d Spacing experimental	38.75	22.44	19.49	14.9		
	d Spacing calculated d_{100}	38.75	38.86	38.98	39.42	0.2934	
	WA d_{100}	38.7929					
	Intensity (cps)	2858	369	223	85		
(10 months aging)	2θ Experimental	2.324	4.032	4.632	6.078		43.86
	2θ (d_{100}) Calculated	2.324	2.327	2.316	2.297	0.0136	
	WA 2θ (d_{100})	2.32334					
	d Spacing experimental	37.99	21.9	19.06	14.53		
	d Spacing calculated d_{100}	37.99	37.93	38.12	38.44	0.2283	

	WA d_{100}	38.00161					
	Intensity (cps)	3434	447	283	85		
(12 months aging)	2θ Experimental	2.277	3.979	4.572	6		44.75
	2θ (d_{100}) Calculated	2.277	2.297	2.286	2.268	0.0126	
	WA 2θ (d_{100})	2.279513					
	d Spacing experimental	38.76	22.19	19.31	14.72		
	d Spacing calculated d_{100}	38.76	38.43	38.62	38.94	0.2164	
	WA d_{100}	38.72088					
	Intensity (cps)	3032	402	247	96		

PXRD conditions: 2θ = 1-7°, scan speed = 0.25, sampling width = 0.02, kV = 30, mA = 15, WA = weighted average value

Table 4S PXRD data of samples of atmospheric conditions analyased for one year

Month	Parameter	d_{100}	d_{110}	d_{200}	d_{210}	Std. Dev.	Unit cell $a_{0,}$ (Å)
Freshly Calcined sample (no aging)	2θ Experimental	2.274	3.957	4.54	6.01		44.62
	2θ (d_{100}) Calculated	2.274	2.284	2.27	2.271	0.0065	
	WA 2θ (d_{100})	2.275					
	d spacing Experimental	38.81	22.31	19.43	14.7		
	d spacing Calculated d_{100}	38.81	38.64	38.86	38.89	0.1113	
	WA d_{100}	38.80					
	Intensity (cps)	4460	538	328	120		
(2 months aging)	2θ Experimental	2.206	3.859	4.421	5.826		45.76
	2θ (d_{100}) Calculated	2.206	2.228	2.21	2.202	0.0114	
	WA 2θ (d_{100})	2.208					
	d spacing Experimental	40.02	22.88	19.97	15.16		
	d spacing Calculated d_{100}	40.02	39.63	39.94	40.11	0.2087	
	WA d_{100}	39.98					
	Intensity (cps)	4550	573	381	130		
(4 months aging)	2θ Experimental	2.384	4.065	4.675	6.13		43.44
	2θ (d_{100}) Calculated	2.384	2.347	2.337	2.317	0.0281	
	WA 2θ (d_{100})	2.378					
	d spacing Experimental	37.03	21.72	18.89	14.41		
	d spacing Calculated d_{100}	37.03	37.62	37.78	38.12	0.4574	
	WA d_{100}	37.13					
	Intensity (cps)	2969	260	180	50		
(6 months aging)	2θ Experimental	2.327	4.021	4.630	6.109		43.79
	2θ (d_{100}) Calculated	2.327	2.321	2.315	2.309	0.0078	
	WA 2θ (d_{100})	2.325					
	d spacing Experimental	37.93	21.96	19.07	14.46		
	d spacing Calculated d_{100}	37.93	38.03	38.14	38.26	0.1404	
	WA d_{100}	37.96					
	Intensity (cps)	2984	394	256	75		
(8 months aging)	2θ Experimental	2.298	4.021	4.626	6.066		44.35
	2θ (d_{100}) Calculated	2.298	2.321	2.313	2.293	0.0133	
	WA 2θ (d_{100})	2.30118					
	d spacing Experimental	38.41	21.96	19.09	14.56		
	d spacing Calculated d_{100}	38.41	38.03	38.18	38.52	0.2198	
	WA d_{100}	38.36049					
	Intensity (cps)	2499	299	197	55		
(10 months aging)	2θ Experimental	2.344	4.051	4.665	6.11		43.48
	2θ (d_{100}) Calculated	2.344	2.339	2.332	2.309	0.0153	

	WA 2θ (d_{100})	2.342219					
	d spacing Experimental	37.66	21.8	18.93	14.44		
	d spacing Calculated d_{100}	37.66	37.76	37.86	38.20	0.2370	
	WA d_{100}	37.69089					
	Intensity (cps)	2358	279	173	48	2358	
(12 months aging)	2θ Experimental	2.328	4.051	4.641	6.097		43.78
	2θ (d_{100}) Calculated	2.328	2.339	2.320	2.304	0.0144	
	WA 2θ (d_{100})	2.328228					
	d spacing Experimental	37.92	21.79	19.03	14.48		
	d spacing Calculated d_{100}	37.92	37.74	38.06	38.31	0.2401	
	WA d_{100}	37.91755					
	Intensity (cps)	2608	382	251	64		

XRD conditions: 2θ = 1-7°, scan speed = 0.25, sampling width = 0.02, kV = 30, mA = 15, WA = weighted average value.