

# NMR and IR study of fluorobenzene and hexafluorobenzene adsorbed on alumina

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## **Supporting information S1.**

### **Nitrogen adsorption data and pore size distribution for neutral alumina.**

Adsorbate Property Factor: 9.530000 A  
 Density Conversion Factor: 0.001547  
 Fraction of Pores Open at Both Ends: 0.000

Average Diameter (Å)	Cumulative Pore Volume (cm³/g)	Smoothed dV/dD Pore Volume (cm³/g·Å)	Cumulative Pore Area (m²/g)	Smoothed dA/dD Pore Area (m²/g·Å)	Smoothed dV/dlog(D) Pore Volume (cm³/g·Å)
2378.6	0.006943	5.7042e-06	0.117	1.1213e-04	2.6216e-02
1276.6	0.015520	1.4799e-05	0.385	5.4520e-04	3.6571e-02
862.3	0.021782	2.6647e-05	0.676	1.4972e-03	4.6550e-02
471.0	0.036355	6.2473e-05	1.913	6.5990e-03	5.6952e-02
306.7	0.046425	9.9301e-05	3.227	1.5487e-02	6.1124e-02
224.5	0.054068	1.3273e-04	4.589	2.7202e-02	6.1435e-02
176.9	0.059831	1.5976e-04	5.892	4.0242e-02	5.9479e-02
145.2	0.064572	1.9124e-04	7.198	5.7655e-02	5.9040e-02
127.4	0.067036	2.1353e-04	7.972	7.1348e-02	5.9960e-02
106.0	0.072498	2.9989e-04	9.996	1.2455e-01	6.8378e-02
88.3	0.079506	6.1991e-04	13.170	3.2225e-01	1.1600e-01
72.0	0.096422	1.9599e-03	22.565	1.1781e+00	2.9853e-01
59.6	0.126174	3.2823e-03	42.529	2.4617e+00	4.1734e-01
50.6	0.155502	3.7268e-03	65.718	3.1483e+00	4.0605e-01
43.7	0.178159	3.4726e-03	86.440	3.3919e+00	3.2876e-01
38.2	0.194599	2.9933e-03	103.656	3.3255e+00	2.4825e-01
33.4	0.206810	2.4868e-03	118.260	3.1487e+00	1.8051e-01
29.7	0.214315	2.1043e-03	128.383	2.9652e+00	1.3660e-01
27.8	0.215701	2.0342e-03	130.375	2.9316e+00	1.2889e-01
27.2	0.217040	1.9659e-03	132.346	2.9009e+00	1.2148e-01
26.5	0.218223	1.9038e-03	134.131	2.8742e+00	1.1491e-01
25.9	0.219353	1.8449e-03	135.875	2.8493e+00	1.0886e-01
25.3	0.220304	1.7832e-03	137.378	2.8235e+00	1.0272e-01
24.7	0.221359	1.7255e-03	139.085	2.7997e+00	9.7027e-02
24.1	0.222349	1.6702e-03	140.727	2.7771e+00	9.1668e-02
23.5	0.223281	1.6189e-03	142.310	2.7585e+00	8.6707e-02
23.0	0.224208	1.5710e-03	143.924	2.7439e+00	8.2048e-02
22.4	0.225032	1.5253e-03	145.396	2.7295e+00	7.7772e-02
21.9	0.225823	1.4809e-03	146.843	2.7134e+00	7.3703e-02
21.3	0.226568	1.4317e-03	148.239	2.6883e+00	6.9529e-02
20.8	0.227334	1.3801e-03	149.711	2.6590e+00	6.5240e-02
20.3	0.228014	1.3308e-03	151.053	2.6303e+00	6.1349e-02
19.8	0.228671	1.2860e-03	152.383	2.6056e+00	5.7875e-02
19.3	0.229275	1.2449e-03	153.635	2.5899e+00	5.4559e-02
18.8	0.229862	1.2063e-03	154.885	2.5789e+00	5.1523e-02
18.3	0.230430	1.1673e-03	156.126	2.5652e+00	4.8523e-02
17.8	0.230962	1.1254e-03	157.324	2.5436e+00	4.5493e-02
17.3	0.231457	1.0815e-03	158.466	2.5073e+00	4.2576e-02
16.6	0.232529	9.8452e-04	161.052	2.4128e+00	3.6555e-02
15.6	0.233374	8.8505e-04	163.213	2.2947e+00	3.1015e-02
14.7	0.234086	7.7225e-04	165.149	2.1389e+00	2.5388e-02
13.8	0.234749	6.7691e-04	167.075	2.0173e+00	2.0777e-02
12.8	0.235363	5.9957e-04	168.992	1.9213e+00	1.7076e-02
11.8	0.235953	5.1143e-04	170.991	1.7996e+00	1.3307e-02
10.7	0.236437	4.6107e-04	172.801	1.8100e+00	1.0832e-02
9.7	0.236886	4.9800e-04	174.664	2.1780e+00	1.0569e-02
8.6	0.237489	6.7417e-04	177.471	3.4099e+00	1.2589e-02
7.0	0.239328	1.6907e-03	187.929	1.0837e+01	2.4721e-02
6.1	0.240103	2.1258e-03	192.984	1.4533e+01	2.9087e-02
5.9	0.240465	2.3134e-03	195.454	1.6227e+01	3.0807e-02
5.7	0.241021	2.5943e-03	199.384	1.8896e+01	3.3221e-02
5.3	0.242371	3.2341e-03	209.547	2.5386e+01	3.7971e-02
5.0	0.243339	3.6668e-03	217.361	3.0371e+01	4.0673e-02
4.4	0.246859	5.1590e-03	249.662	5.3167e+01	4.7725e-02
3.6	0.250979	6.2517e-03	295.146	7.4449e+01	4.7855e-02
3.0	0.254761	5.3123e-03	345.928	7.7634e+01	3.3210e-02
2.4	0.256633	1.6755e-03	377.655	3.6702e+01	8.0885e-03

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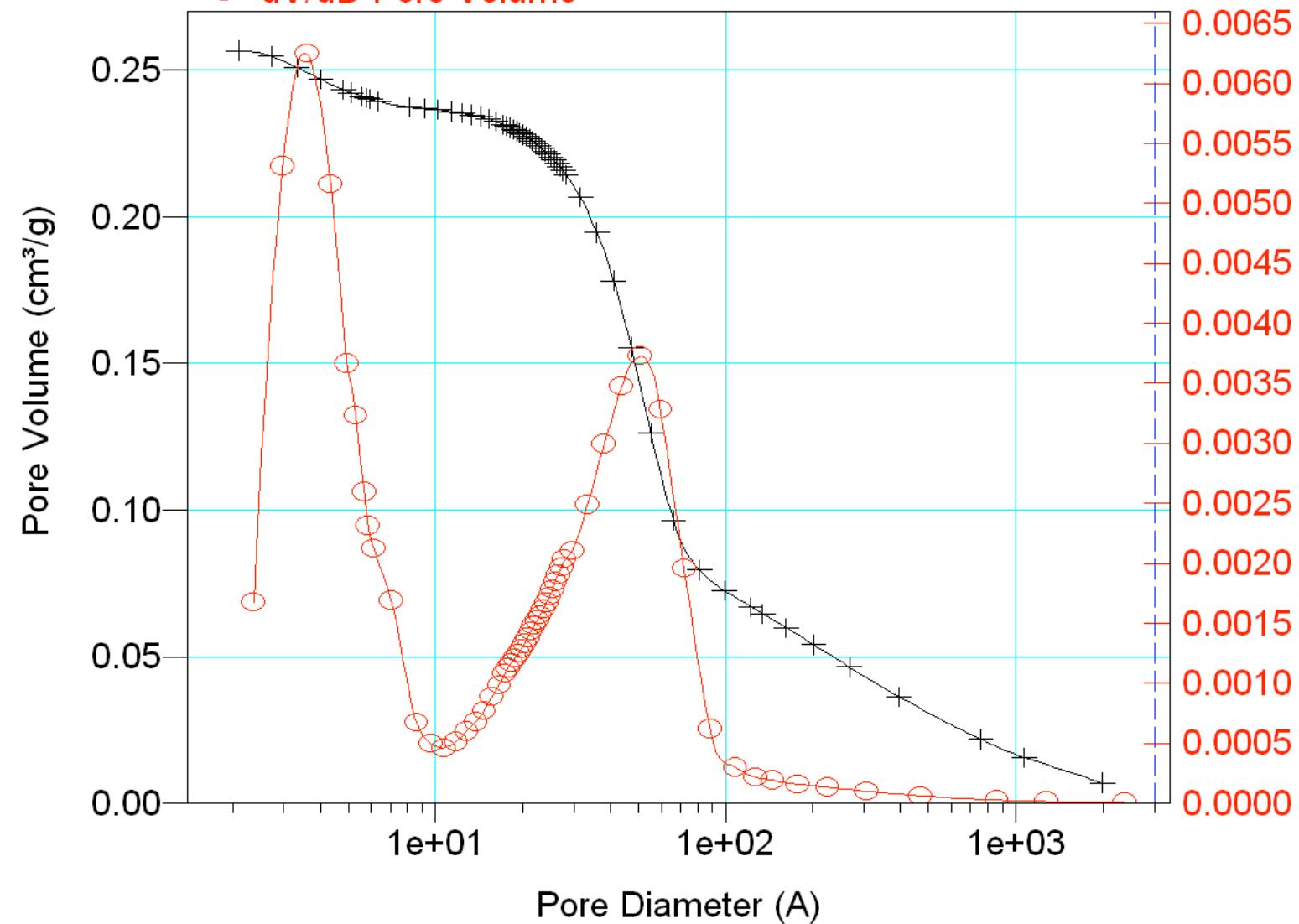
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## BJH Adsorption Cumulative Pore Volume

+ Cumulative Pore Volume

○ dV/dD Pore Volume



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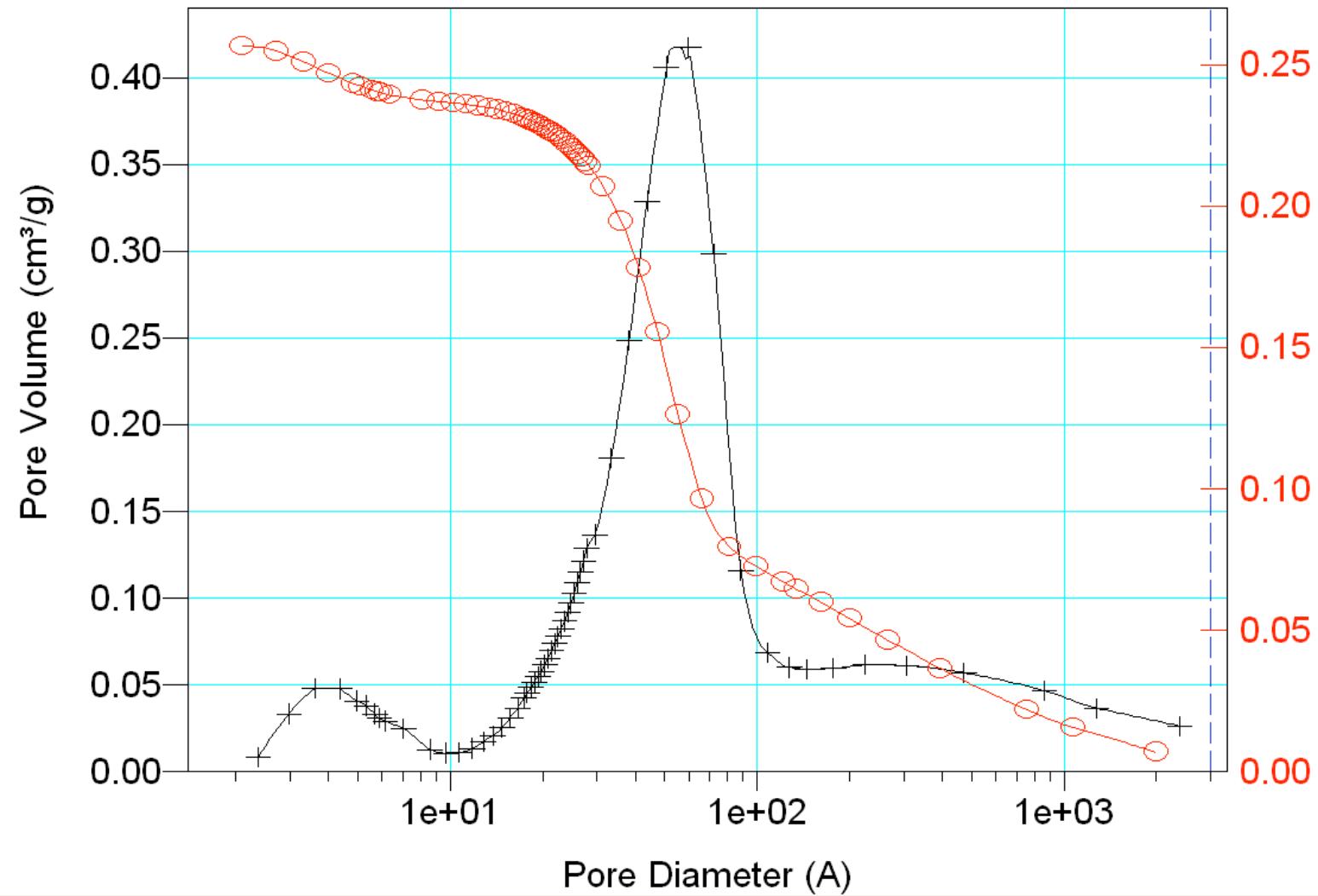
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### BJH Adsorption $dV/d\log(D)$ Pore Volume (smoothed)

+ dV/dlog(D) Pore Volume

○ Cumulative Pore Volume



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