

Microporous co-polymers for increased gas selectivity

Robert Dawson,^{*a} Matthew Corker,^a Thanchanok Ratvijitvech,^a Andrew I. Cooper^a and Dave J. Adams^{*a}

Contents

Elemental Analysis

FTIR

BET plots

CO₂ uptakes and selectivity

1. Elemental Analysis

Table S1. Example Elemental Analysis for Benzene/Aniline

% Aniline	% Benzene	Expected % C	Found % C	Expected % H	Found % H	Expected % N	Found % N
0	100	94.08	83.66	5.92	5.34	0.00	0.00
10	90	92.72	83.12	5.93	5.36	1.35	1.11
20	80	91.39	80.51	5.94	5.26	2.66	1.96
30	70	90.10	77.59	5.95	5.18	3.94	2.81
40	60	88.85	74.97	5.97	5.11	5.18	3.90
50	50	87.64	74.43	5.98	5.61	6.39	5.54
60	40	86.45	70.28	5.99	5.45	7.56	6.56
70	30	85.30	65.59	6.00	5.30	8.70	7.41
80	20	84.18	64.23	6.00	5.14	9.82	7.88
90	10	83.09	64.18	6.01	5.11	10.90	9.40
100	0	82.02	62.90	6.02	5.06	11.96	9.40

Elemental Analysis of the networks was averaged over three repeat reactions

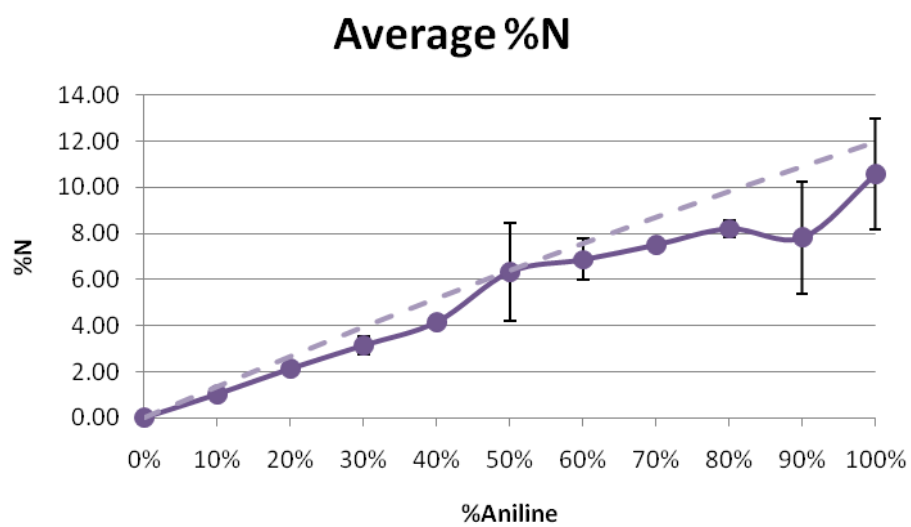


Fig S1. Average nitrogen content of three repeat syntheses. Dotted line represents theoretical nitrogen content.

2. FTIR

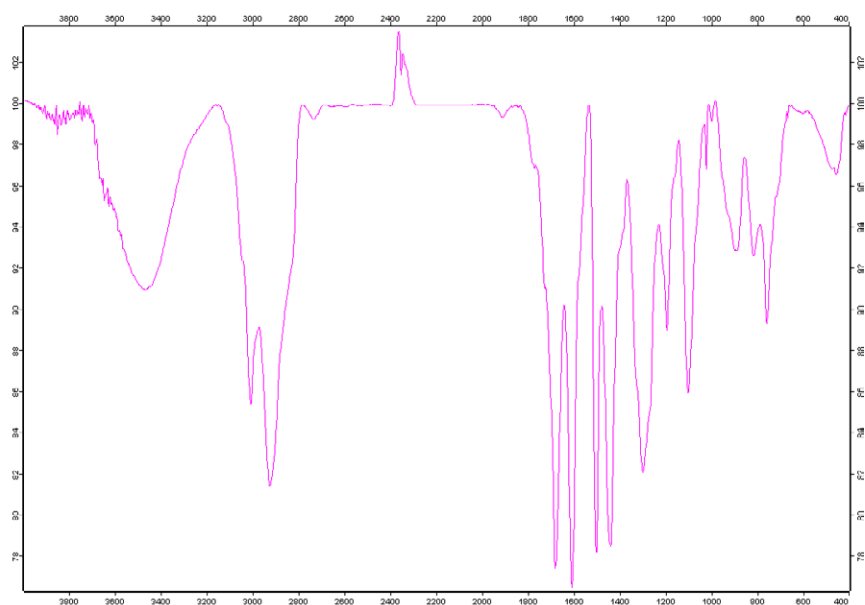


Fig. S2.1 FTIR spectrum of 0 % Aniline

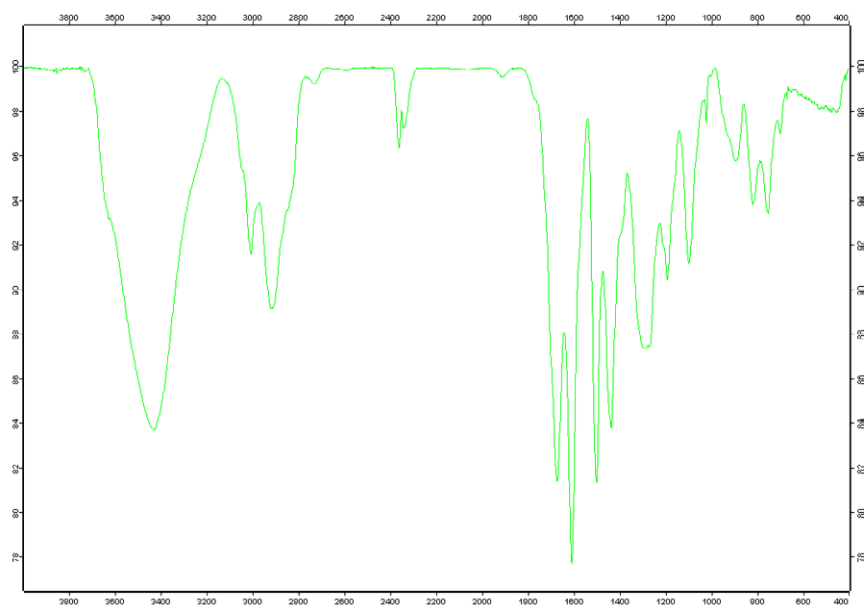


Fig. S2.2 FTIR spectrum of 10 % Aniline

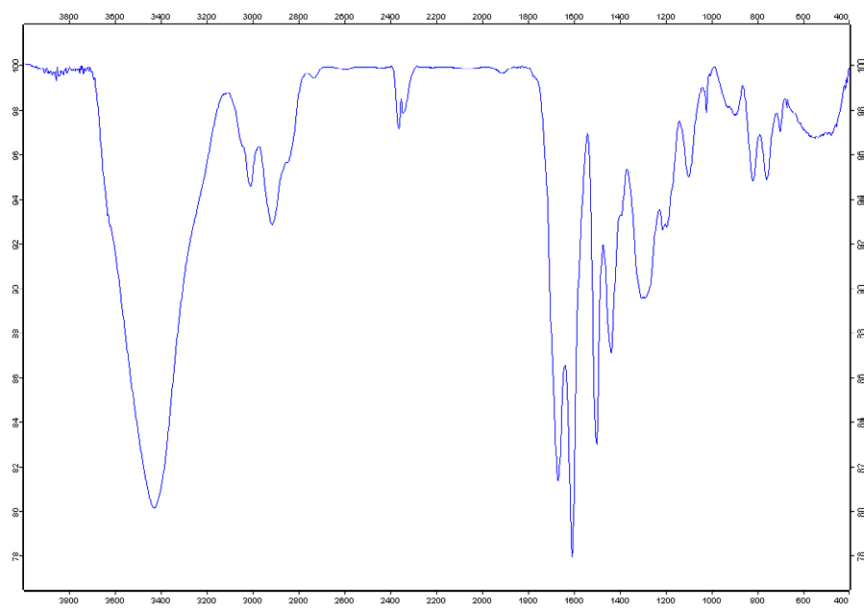


Fig. S2.3 FTIR spectrum of 20 % Aniline

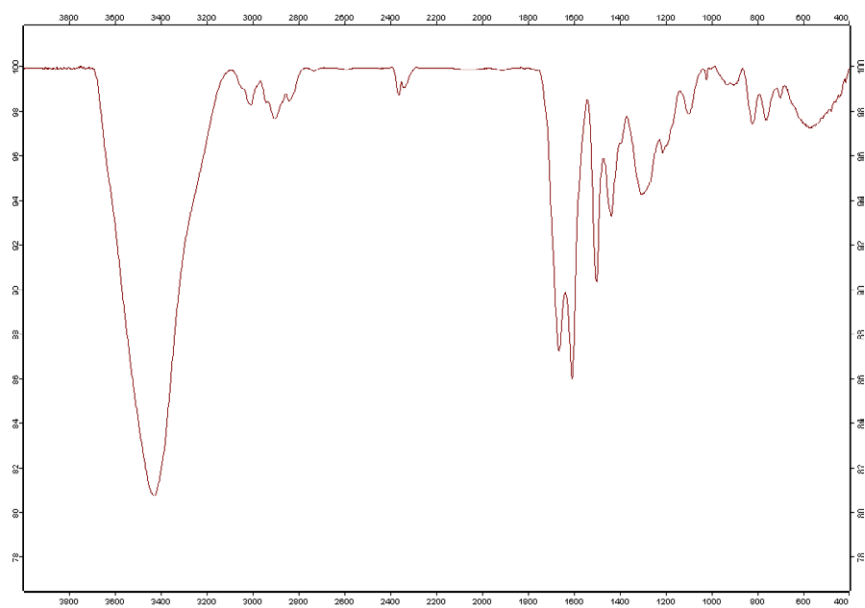


Fig. S2.4 FTIR spectrum of 30 % Aniline

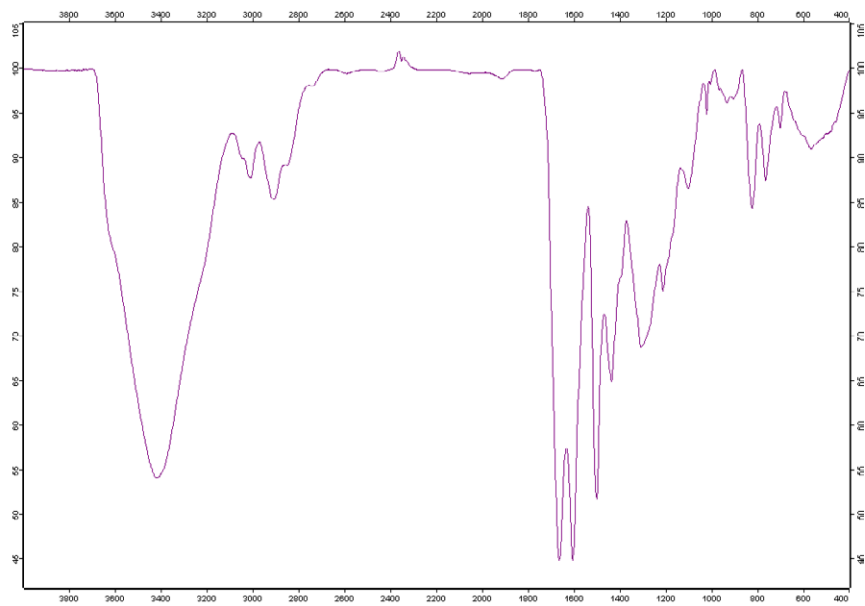


Fig. S2.5 FTIR spectrum of 40 % Aniline

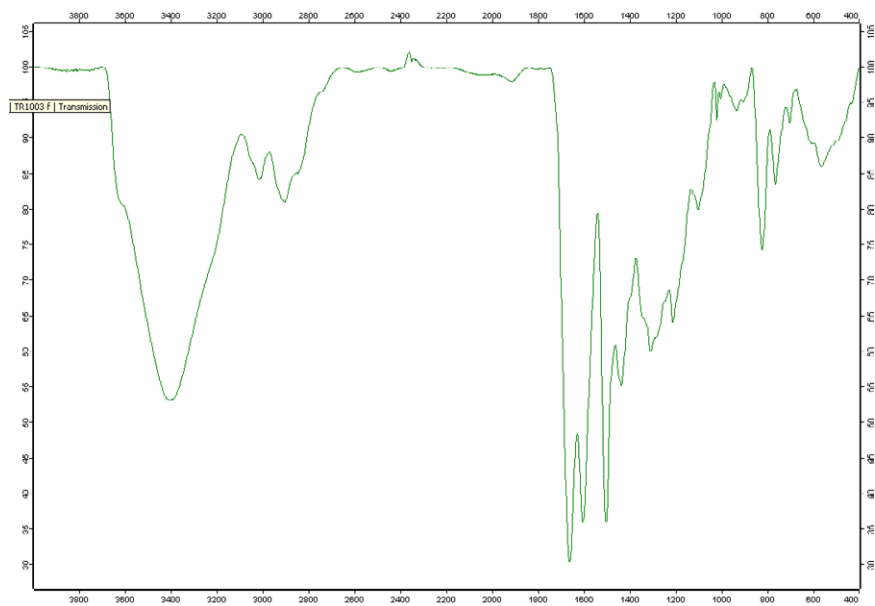


Fig. S2.6 FTIR spectrum of 50 % Aniline

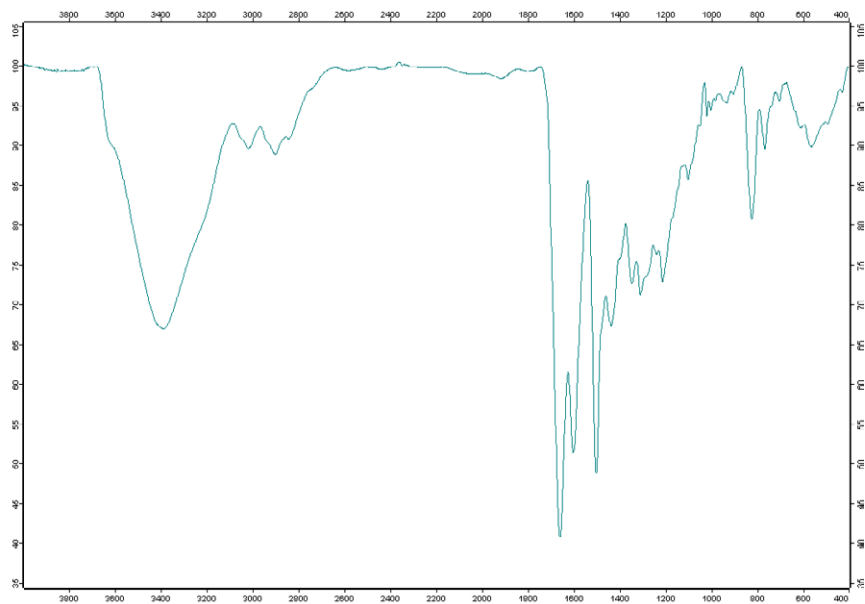


Fig. S2.7 FTIR spectrum of 60 % Aniline

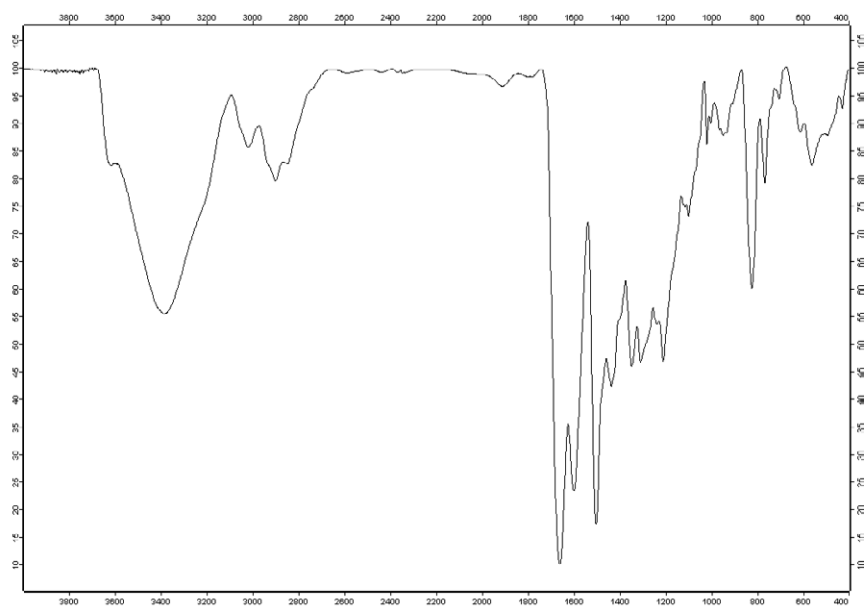


Fig. S2.8 FTIR spectrum of 70 % Aniline

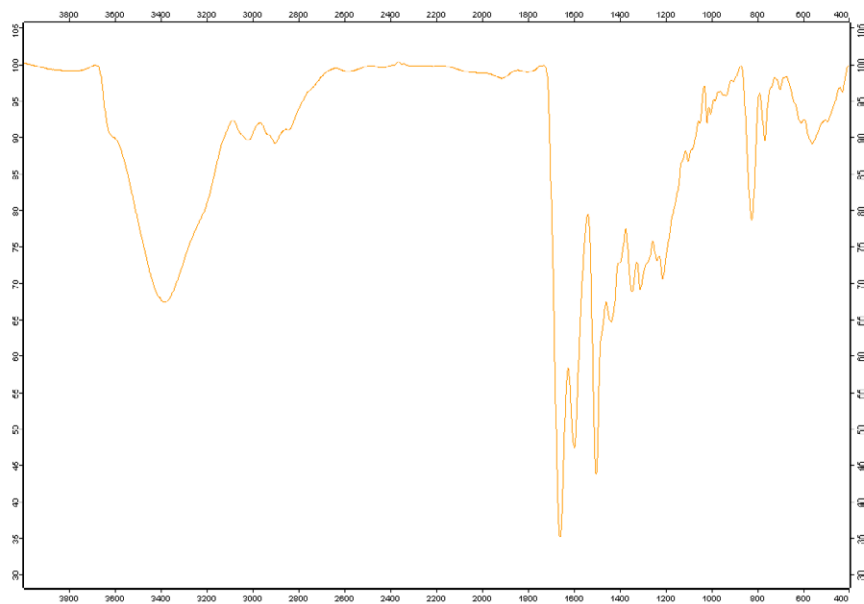


Fig. S2.9 FTIR spectrum of 80 % Aniline

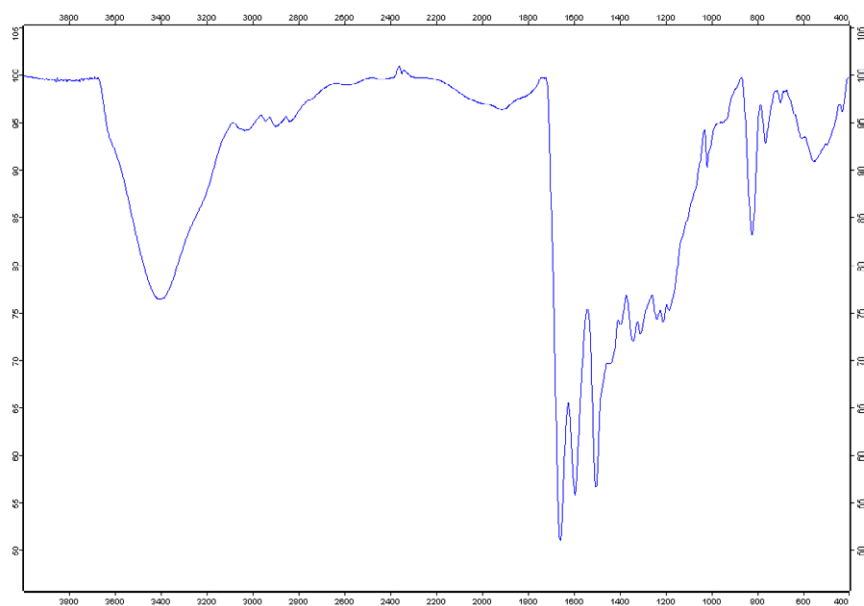


Fig. S2.10 FTIR spectrum of 90 % Aniline

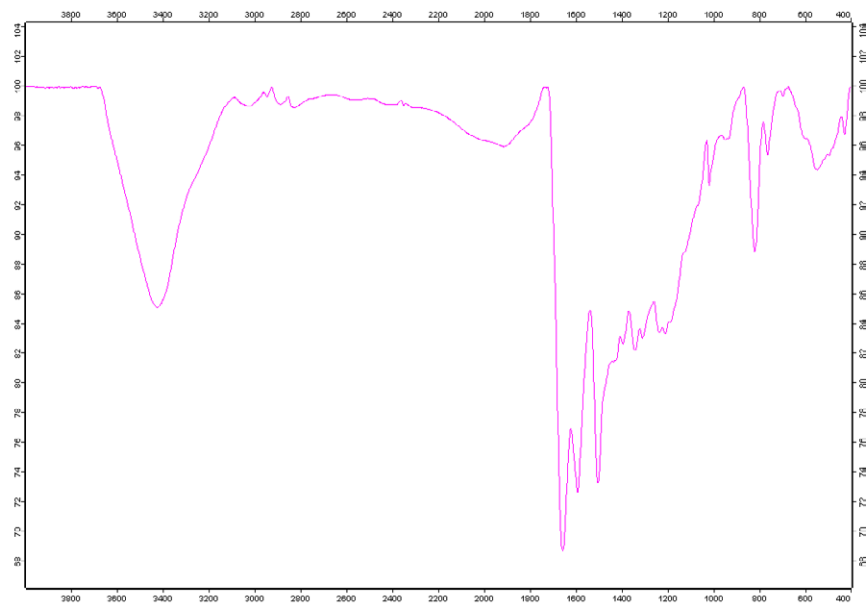


Fig. S2.11 FTIR spectrum of 100 % Aniline

3. BET plots

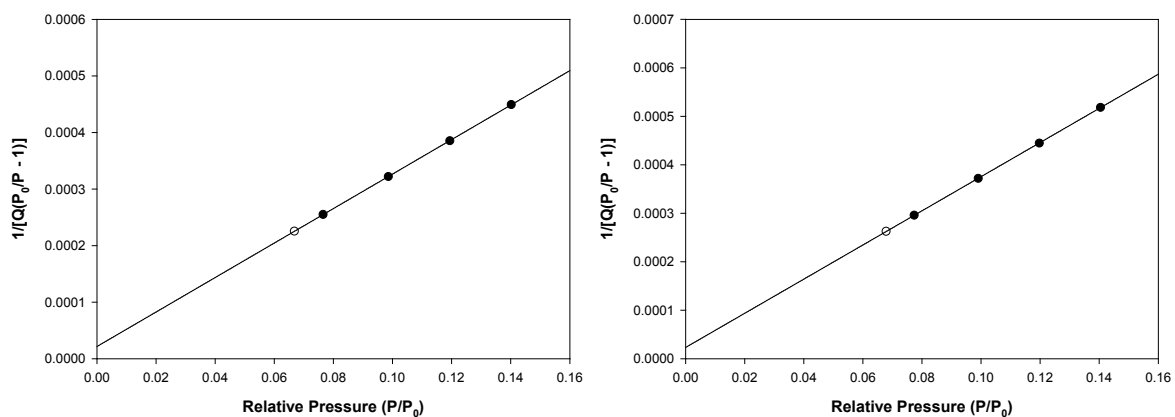


Figure 3.1 BET plots of 0 % (left) and 10 % Aniline (right) networks

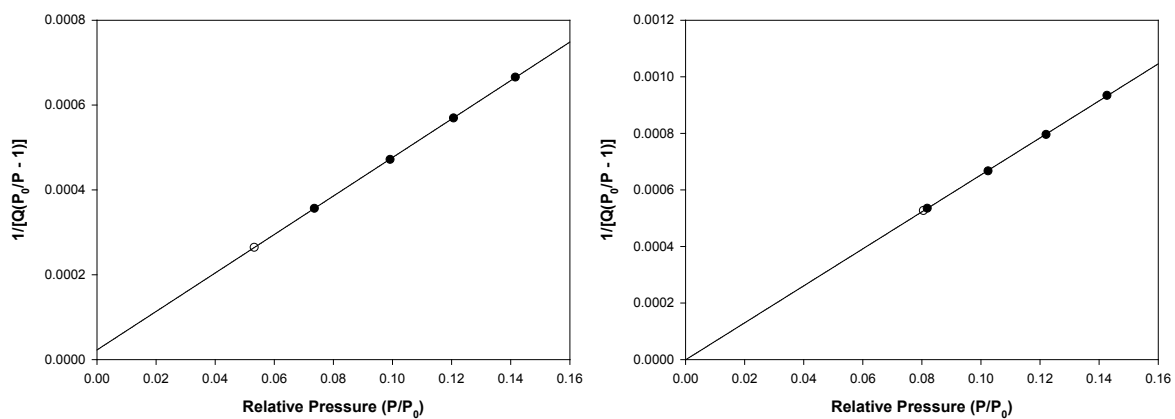


Figure 3.2 BET plots of 20 % (left) and 30 % Aniline (right) networks

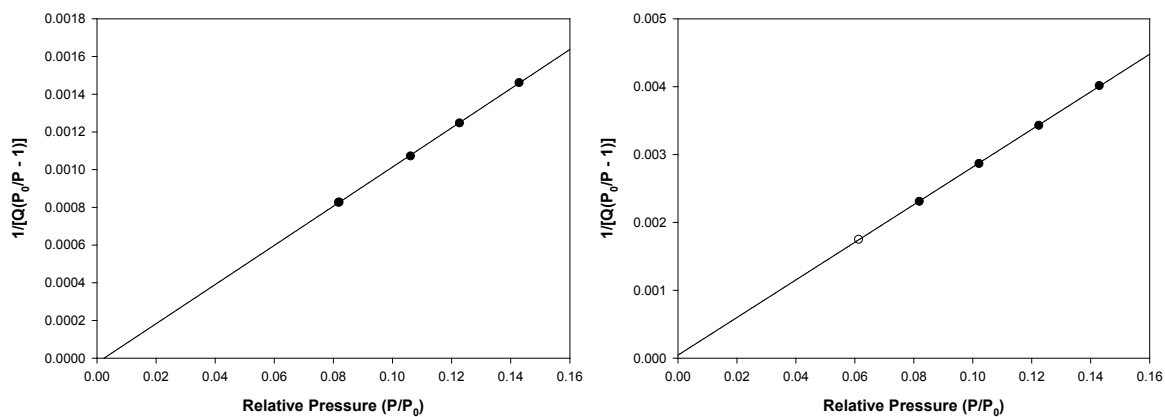


Figure 3.3 BET plots of 40 % (left) and 50 % Aniline (right) networks

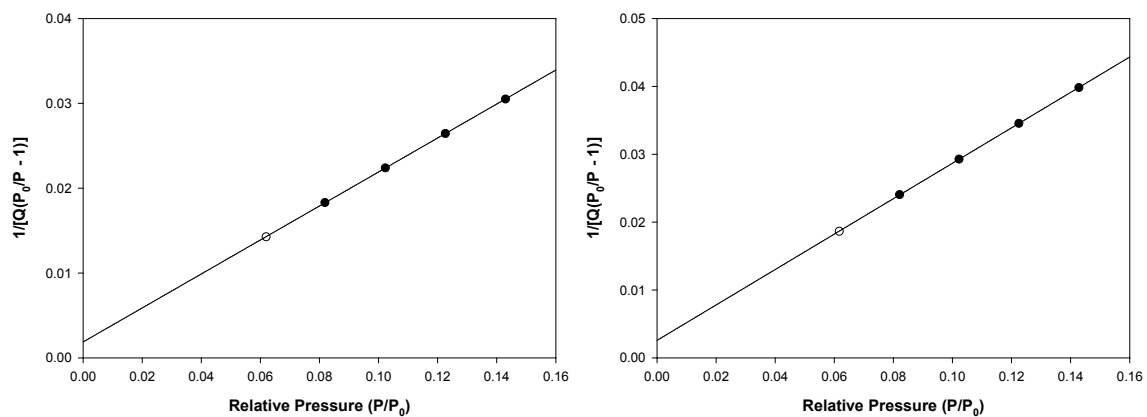


Figure 3.4 BET plots of 60 % (left) and 70 % Aniline (right) networks

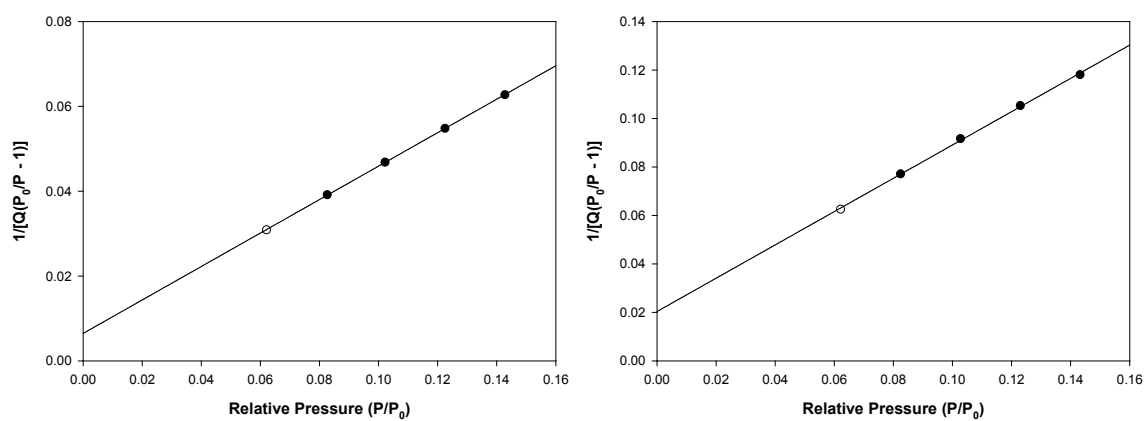


Figure 3.5 BET plots of 80 % (left) and 90 % Aniline (right) networks

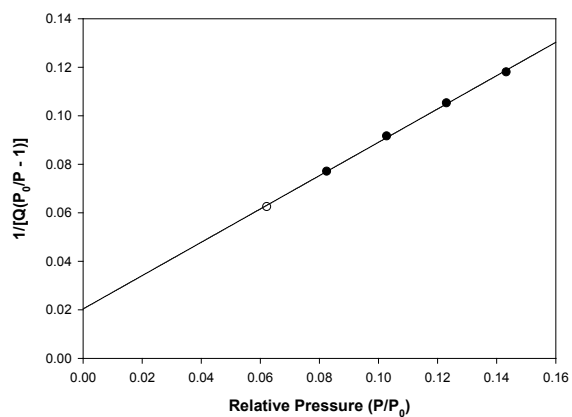


Figure 3.6 BET plots of 100 % Aniline network

4. CO₂ uptakes and CO₂/N₂ selectivity

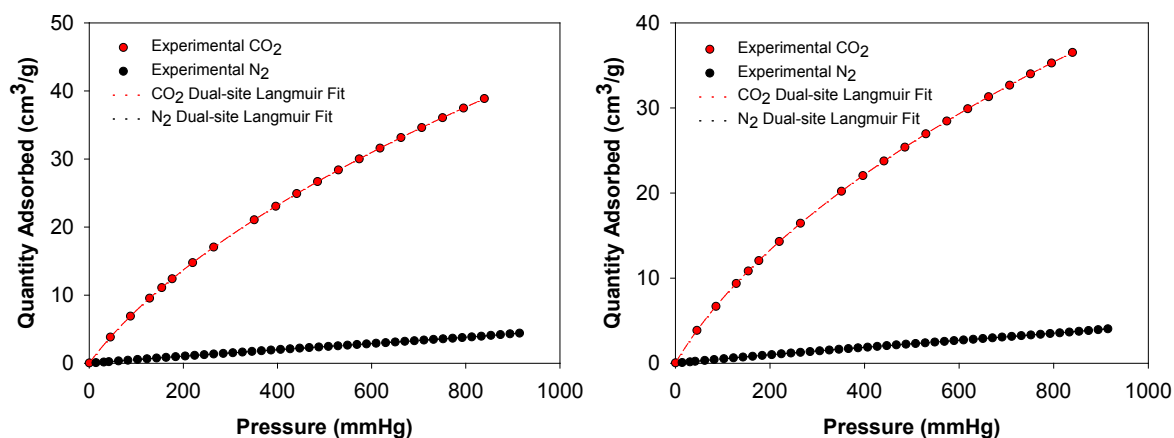


Figure 4.1 CO₂ and N₂ uptakes of 0 % (left) and 10 % Aniline (right) networks at 300 K

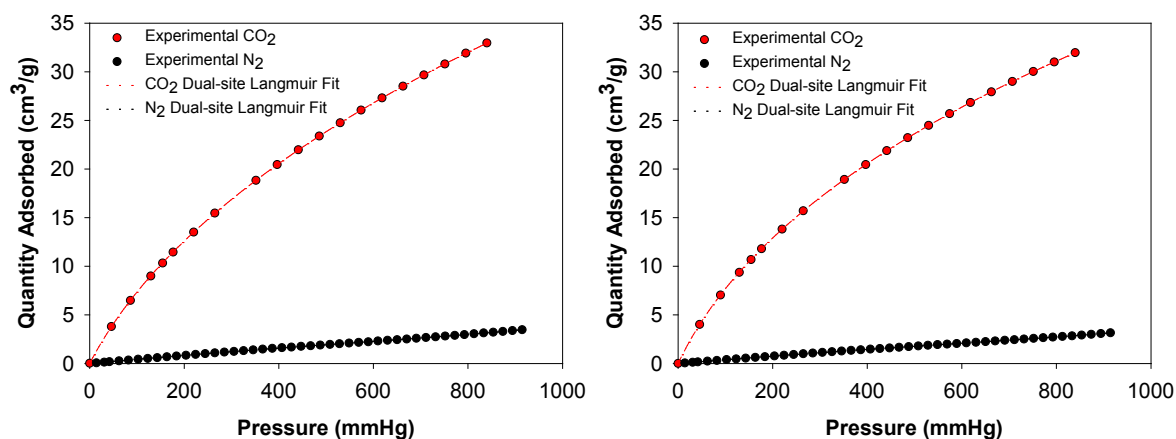


Figure 4.2 CO₂ and N₂ uptakes of 20 % (left) and 30 % Aniline (right) networks at 300 K

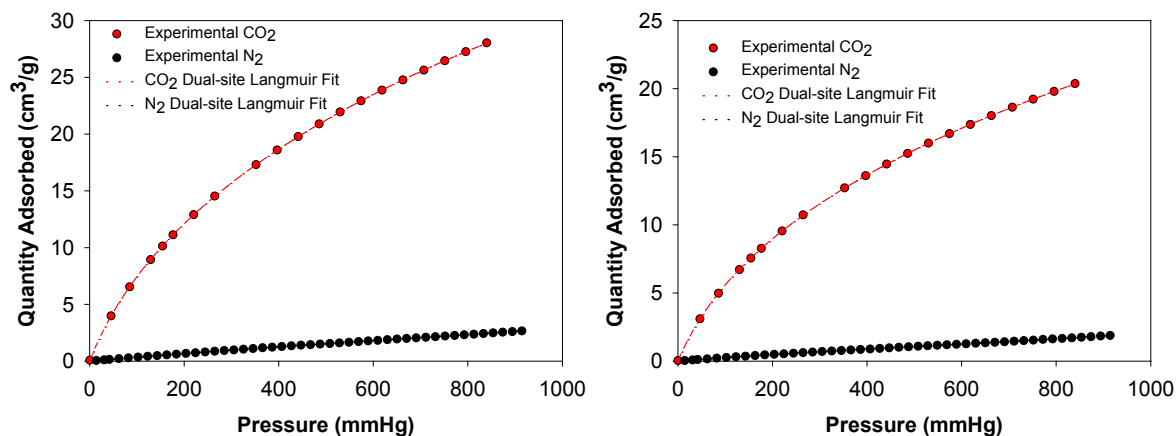


Figure 4.3 CO₂ and N₂ uptakes of 40 % (left) and 50 % Aniline (right) networks at 300 K

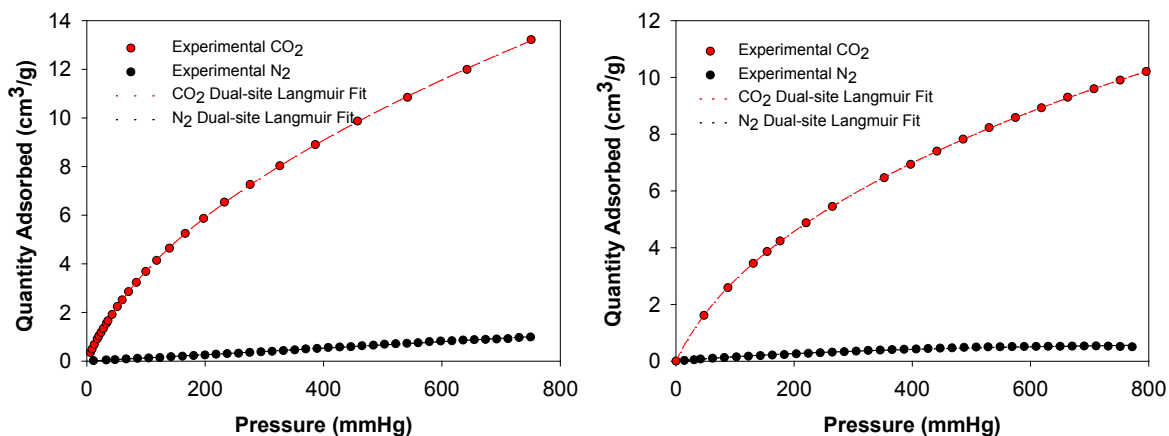


Figure 4.4 CO₂ and N₂ uptakes of 60 % (left) and 70 % Aniline (right) networks at 300 K

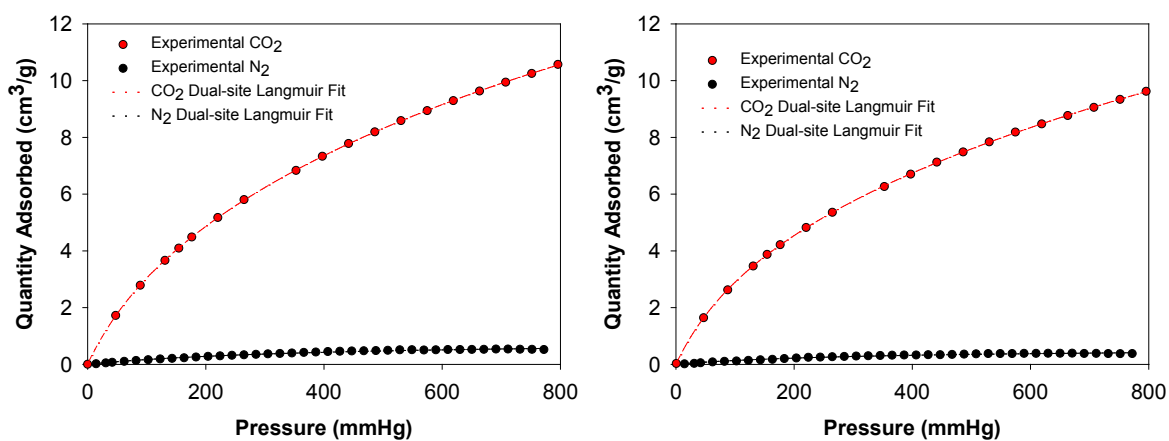


Figure 4.5 CO₂ and N₂ uptakes of 80 % (left) and 90 % Aniline (right) networks at 300 K

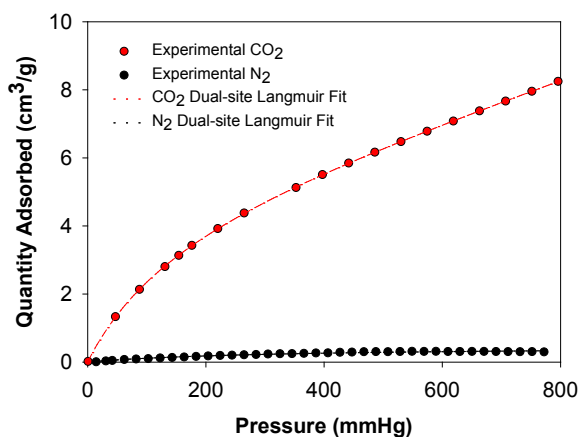


Figure 4.6 CO₂ and N₂ uptakes of 100 % Aniline network at 300 K

5. Benzene/aniline polymer mixtures

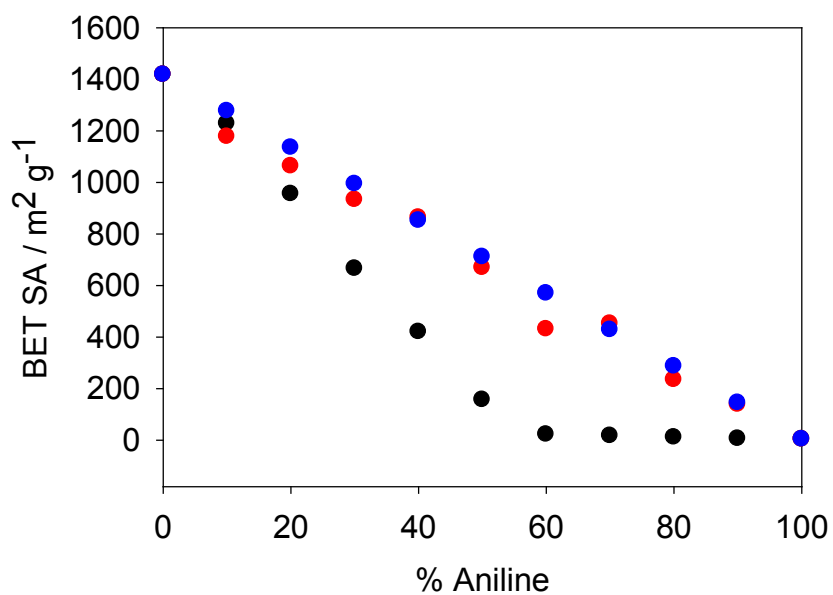


Figure 5 BET surface areas for copolymers (black data), physical admixtures of pure aniline and pure benzene networks (red data) and expected data calculated from the BET surface areas of the pure benzene and pure aniline networks (blue data).

6. Solid state NMR

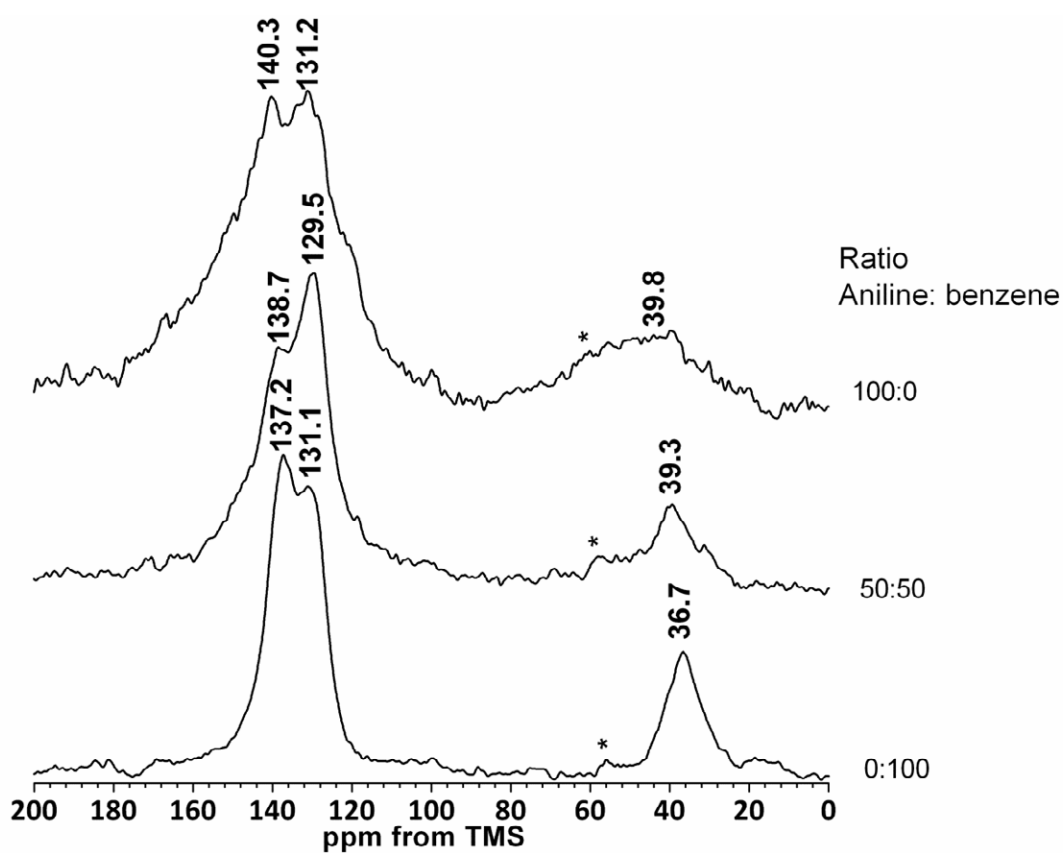


Figure 6 ^{13}C { ^1H } MAS solid-state NMR spectra of networks. Spectra recorded at an MAS rate of 10 kHz. Asterisks denote spinning sidebands. Chemical shifts are given in ppm.

7. NL-DFT pore size distributions

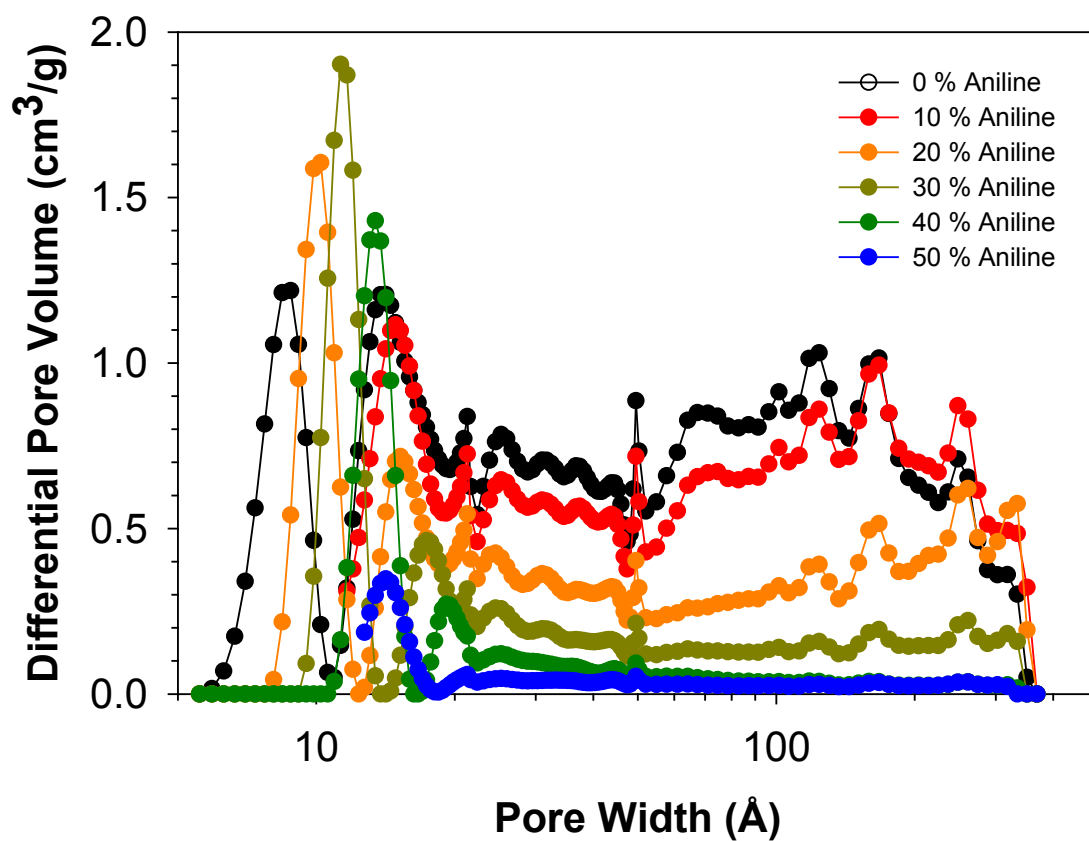


Figure 7 NL-DFT pore size distributions for 0 – 50 % Aniline networks calculated using a cylindrical pore model for Pillared Clay.

Table 7 Surface area and pore volume analysis

% Aniline	Average S_{BET} (m ² /g)	V_{tot} (cm ³ /g)	$V_{0.1}$ (cm ³ /g)	$V_{0.1/\text{tot}}$
0	1289 ± 156	1.47	0.52	0.35
10	1097 ± 123	1.27	0.45	0.35
20	757 ± 181	1.31	0.35	0.27
30	481 ± 209	0.65	0.26	0.40
40	238 ± 161	0.26	0.16	0.62
50	152 ± 142	0.13	0.05	0.38