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APPENDICES

Appendix A Sanderson's Intermediate Electronegativity (S_{int}) Calculation

Sanderson's intermediate electronegativity (S_{int}) was calculated following Equation A1 to represent the strength of the adsorbent acidity (It is noted that the higher S_{int} indicates high electron-accepting ability and strong adsorbent acidity (Bathomeuf, 1996).):

$$S_{int} = \left(\prod_i S_i^{n_i} \right)^{1/(\sum n_i)}, \quad (A1)$$

where S_i is the Sanderson's electronegativity of the atom, and n_i is the stoichiometric of the atom in a unit cell of adsorbent.

For the Na-faujasite zeolites with a formula of $Na_p(SiO_2)_r(AlO_2)_s$, the S_{int} can be calculated by

$$S_{int} = (S_{Na}^p S_{Si}^r S_{Al}^s S_O^{2(r+s)})^{1/(p+r+s+2(r+s))} \quad (A2)$$

The S_{int} of Na, Si, Al, and O used in the calculation for this experiment are shown in Table A1. The chemical composition of the zeolites is shown in Table A2, together with their calculated Sanderson's intermediate electronegativity (S_{int}).

Table A1 Sanderson's intermediate electronegativity (S_{int}) (Barthomeuf, 1996)

	Na	Si	Al	O
Sanderson's intermediate electronegativity (S_{int})	0.70	2.84	2.22	5.21

Table A2 Chemical composition and Sanderson's intermediate electronegativity (S_{int}) of the employed Na-faujasite zeolites

Adsorbent	Chemical Composition	Sanderson's intermediate electronegativity (S_{int})
2.0NaX	$Na_{96}(AlO_2)_{96}(SiO_2)_{96}$	3.175
2.5NaX	$Na_{84}(AlO_2)_{84}(SiO_2)_{108}$	3.249
5.0NaY	$Na_{53}(AlO_2)_{53}(SiO_2)_{139}$	3.462
12.0NaY	$Na_{25}(AlO_2)_{25}(SiO_2)_{167}$	3.687

Appendix B Basicity Definition

The basicities of methylbenzenes were first measured by McCaulay and Lien, 1951 by means of competitive extraction experiments in which mixtures of methylbenzenes competed for a limited amount of acid (HF-BF₃). The solubility of aromatic in HF increases with its basicity. It was proposed in their work that the reaction of complex formation is the sum of the following two steps.



The stability of the methylbenzene cation formed in an HF-BF₃ medium varies greatly with the number and orientation of the methyl substituents. These differences in stability could be accounted for by postulating structures for the cation similar to those commonly assigned to intermediates in aromatic substitution reactions.

To obtain the basicity of one methylbenzene relative to benzene, a mixture of that methylbenzene and benzene has to be used as a reactant for the extraction experiment. The relative η basicities of methylbenzenes to benzene are shown in Table B1.

Table B1 Relative η basicities of benzene and methylbenzenes (Olah, 1971)

	Relative η -complex stability
Benzene	1
Ethylbenzene (EB)	1.5
Toluene	1.5
p-Diethylbenzene (pDEB)	1.55
p-Xylene	1.6
o-Xylene	1.8
m-Xylene	2.0

Appendix C Selectivity Calculation

A schematic pulse test is shown in Figure B1. Each component peak was indexed on the volume scale at the midpoint of the chord at 50% peak height. The net retention volume (NRV) of each component was measured using the tracer peak as the zero origin.

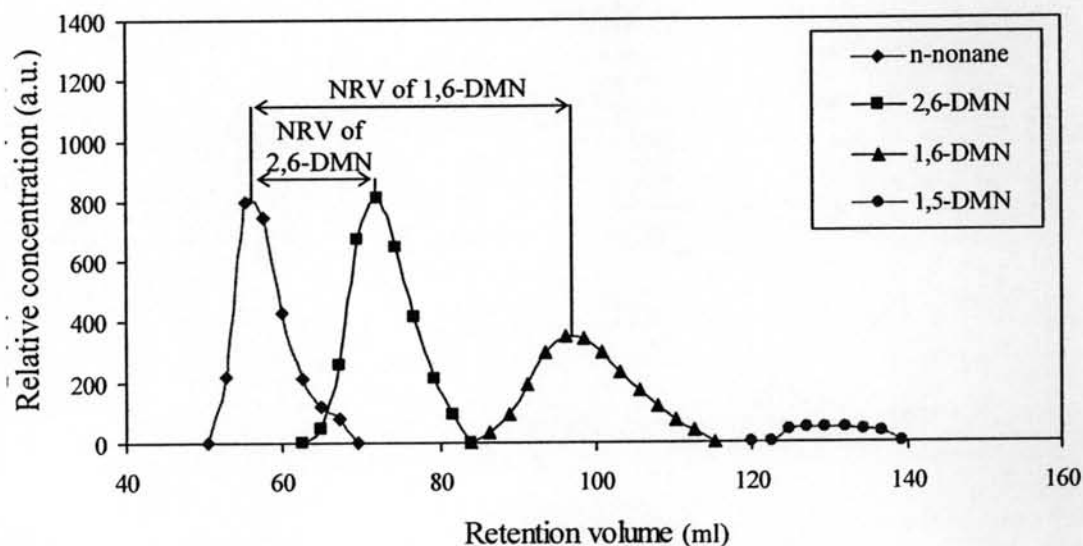


Figure.C1 Schematic of dynamic adsorption: Multi-component pulse test.

The selectivity of 1,6-DMN with respect to 2,6-DMN can be calculated from the ratio of 1,6-DMN to 2,6-DMN as in Equation B1:

$$\alpha_{1,6-DMN/2,6-DMN} = \frac{NRV \text{ of } 1,6-DMN}{NRV \text{ of } 2,6-DMN} \quad (B1)$$

The selectivity of 1,5-DMN with respect to 2,6-DMN can be calculated in the same way. Because the NRV of any component is ideally proportional to its distribution coefficient, i.e. its concentration in the adsorbed phase divided by its concentration in the unadsorbed phase, the calculated quantity is essentially equivalent to selectivity as defined for separations carried out in a liquid system (Kulprathipanja *et al.*, 2002).

Appendix D Selectivity of 1,5-DMN and 1,6-DMN with respect to 2,6-DMN from the Dynamic Adsorption Experiment on Different Adsorbents

Table D1 Selectivity of 1,5-DMN and 1,6-DMN with respect to 2,6-DMN from the dynamic adsorption experiment on 2.5NaX adsorbent

Desorbent	Selectivity	
	1,5-DMN/2,6-DMN	1,6-DMN/2,6-DMN
Benzene	N/A	1.159
Ethylbenzene	4.720	1.582
Toluene	4.690	2.060
pDEB	N/A	2.927
p-xylene	7.386	2.283
o-xylene	5.295	1.744
m-xylene	3.911	1.529

Table D2 Selectivity of 1,5-DMN and 1,6-DMN with respect to 2,6-DMN from the dynamic adsorption experiment on 5.0NaY adsorbent

Desorbent	Selectivity	
	1,5-DMN/2,6-DMN	1,6-DMN/2,6-DMN
Benzene	2.495	2.091
Ethylbenzene	4.286	3.227
Toluene	3.661	5.170
pDEB	4.837	2.718
p-xylene	4.413	2.771
o-xylene	2.963	3.243
m-xylene	2.972	3.193

Table D3 Selectivity of 1,5-DMN and 1,6-DMN with respect to 2,6-DMN from the dynamic adsorption experiment on 2.0NaX adsorbent

Desorbent	Selectivity	
	1,5-DMN/2,6-DMN	1,6-DMN/2,6-DMN
Ethylbenzene	3.5657	1.3321
Toluene	3.3968	1.2128
p-xylene	5.6092	2.4056

Table D4 Selectivity of 1,5-DMN and 1,6-DMN with respect to 2,6-DMN from the dynamic adsorption experiment on 12.0NaY adsorbent

Desorbent	Selectivity	
	1,5-DMN/2,6-DMN	1,6-DMN/2,6-DMN
Ethylbenzene	3.9807	1.8716
Toluene	4.3978	1.9875
p-xylene	4.6447	2.1149

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