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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).):

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

$$S_{int} = (S_{Na}^p S_{Si}^r S_{Al}^r S_O^{2(r+s)})^{1/[p+r+s+2(r+s)]}$$
(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}) for the various zeolites considered

Sample	Chemical composition	Cationic radius (Å)	Sanderson's intermediate electronegativity(S_{int})
LiY	$Li_{22}Na_{31}(AlO_2)_{53}(SiO_2)_{139}$	0.76	3.587
NaY	$Na_{53}(AlO_2)_{53}(SiO_2)_{139}$	1.02	3.58
KY	$K_{51}Na_2(AlO_2)_{53}(SiO_2)_{139}$	1.38	3.435
RbY	$Rb_{47}Na_6(AlO_2)_{53}(SiO_2)_{139}$	1.52	3.409
CsY	$Cs_{49}Na_4(AlO_2)_{53}(SiO_2)_{139}$	1.67	3.334
LiX	$Li_{20}Na_{64}(AlO_2)_{84}(SiO_2)_{108}$	0.76	3.284
NaX	$Na_{84}(AlO_2)_{84}(SiO_2)_{108}$	1.02	3.278
KX	$K_{82}Na_2(AlO_2)_{84}(SiO_2)_{108}$	1.38	3.076
RbX	$Rb_{71}Na_{13}(AlO_2)_{84}(SiO_2)_{108}$	1.52	3.052
CsX	$Cs_{73}Na_{11}(AlO_2)_{84}(SiO_2)_{108}$	1.67	2.962

Appendix B Adsorption capacities of single component system and total adsorption capacities of binary system

Table B1 Adsorption capacities of single component system and total adsorption capacities of binary system on various cation exchanged X and Y type zeolite at 30°C

Adsorbent	Adsorption capacities (g/g adsorbent)				
	Single component System		Binary component system		
	m-CNB	p-CNB	m-CNB	p-CNB	m-CNB+p-CNB
LiY	0.3104	0.2756	0.1695	0.1279	0.2974
NaY	0.3026	0.2848	0.1603	0.1100	0.2703
KY	0.2652	0.2547	0.1456	0.0975	0.2431
RbY	0.2317	0.2011	0.1065	0.0968	0.2033
CsY	0.1947	0.1283	0.0772	0.0836	0.1608
LiX	0.3524	0.3259	0.2097	0.1352	0.3449
NaX	0.2841	0.2913	0.1578	0.1036	0.2614
KX	0.2419	0.2402	0.1329	0.0851	0.2180
RbX	0.1913	0.1942	0.1020	0.0837	0.1857
CsX	0.1722	0.1760	0.0872	0.0788	0.1660

Table B2 Adsorption capacities of *m*-CNB and *p*-CNB on various zeolite types

Adsorbent	Adsorption capacities (g/g adsorbent)		K		R^2	
	m-CNB	*p*-CNB	*m*-CNB	*p*-CNB	*m*-CNB	*p*-CNB
LiY	0.3104	0.2756	1196	827	0.9891	0.9939
NaY	0.3026	0.2848	1789	166	0.9997	0.9958
KY	0.2652	0.2547	753	480	0.9986	0.9937
RbY	0.2317	0.2011	1419	1569	0.9988	0.9995
CsY	0.1947	0.1283	1679	13627	0.9959	0.9995
LiX	0.3524	0.3259	1805	1005	0.9988	0.9938
NaX	0.2841	0.2913	5360	191˙	0.9991	0.9998
KX	0.2419	0.2402	7335	417	0.9975	0.9997
RbX	0.1913	0.1942	638	1640.	0.9995	0.9987
CsX	0.1722	0.1760	248	8666	0.9947	0.9984

Table B3 Adsorption capacities of desorbent on NaY zeolites

Desorbent	Adsorption capacities (g/g adsorbent)	K	R^2
Benzene	0.1718	53	0.9957
Toluene	0.1769	22	0.9771
o-Xylene	0.1996	27	0.9971
o-Dichlorobenzene	0.2251	273	0.999
Nitrobenzene	0.2600	740	0.9975

Appendix C Selectivity calculation from binary component system

The *m*-CNB selectivity with respect to *p*-CNB was determined as

$$\alpha_{M/P} = \frac{X_M / X_P}{Y_M / Y_P}$$

(C.1)

where X_M is the mole fraction of *m*-CNB in adsorbed phase.

X_P is the mole fraction of *p*-CNB in adsorbed phase.

Y_M is the mole fraction of *m*-CNB in fluid phase.

Y_P is the mole fraction of *p*-CNB in fluid phase.

Appendix D Selectivity of *m*-CNB with respect to *p*-CNB from binary component system on various zeolite types

Table D1 Selectivity of *m*-CNB with respect to *p*-CNB on various zeolite types

Adsorbent	*m*-CNB/*p*-CNB selectivity	
	At low concentration	At high concentration
LiY	2.36	1.63
NaY	4.37	2.08
KY	2.65	2.03
RbY	1.19	1.11
CsY	0.90	0.85
LiX	2.49	2.03
NaX	4.38	1.93
KX	2.9	1.87
RbX	1.70	1.29
CsX	1.59	1.20

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