Monovalent and Bivalent Cations Exchange Isotherms for Faujasites X and Y

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Supporting Information

Without supposing ideality, Equation 13 becomes:

$$Z_{A,j} = \frac{K_j^{1/v} S_A}{K_j^{1/v} S_A + (1 - S_A) \times \Gamma}$$

And Equation 14 becomes:

$$Z_{A,j}^{*} = \frac{\frac{K_j}{N_T} S_A}{\frac{K_j}{N_T} S_A + (1 - S_A)^2 \times \Gamma}$$

with $\Gamma = \left(\frac{\gamma_B}{\gamma_A}\right)^v$. To calculate γ_i, an expanded Hückel model is used:

$$Ln\gamma_i = \frac{-A_\gamma v_i^2 \sqrt{I}}{1 + \beta a \sqrt{I}} + c_i I$$

I is the ionic strength calculated with the following formula:

$$I = \frac{1}{2} \sum_{i=1}^{i} v_i^2 m_i$$

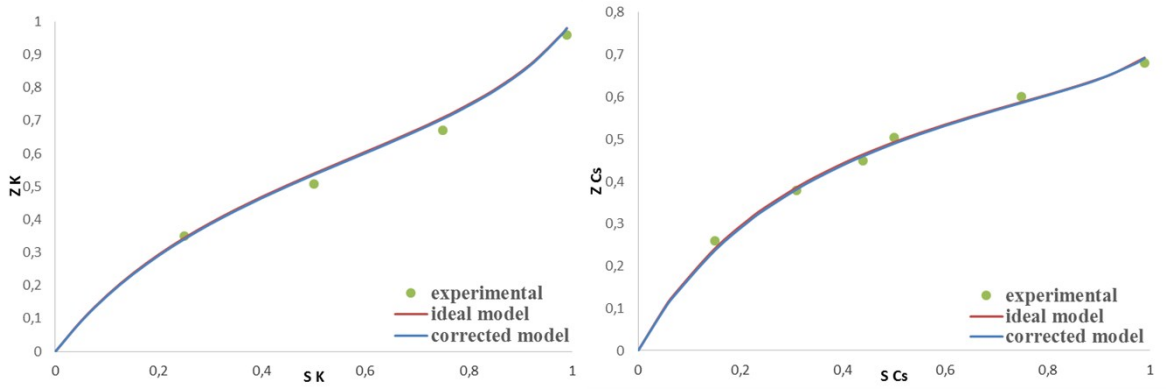

Figure S1. Comparison between ideal and corrected exchange isotherm models (left: K-Na-Y, right: Cs-Na-Y)

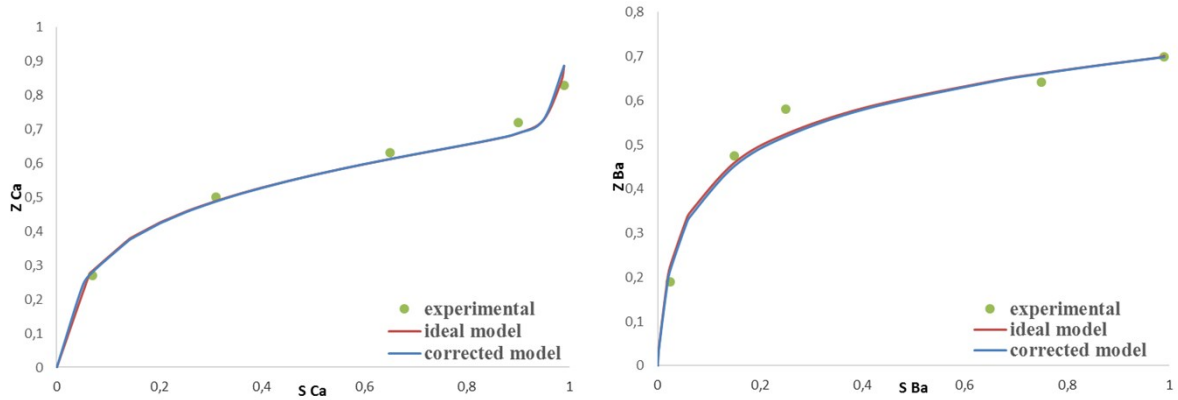

Figure S2. Comparison between ideal and corrected exchange isotherm models (left: Ca-Na-Y, right: Ba-Na-Y)

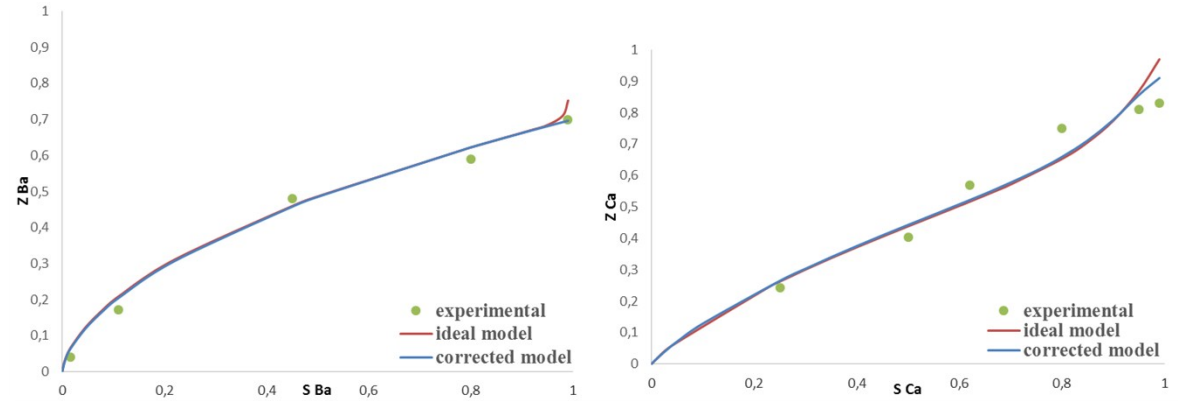

Figure S3. Comparison between ideal and corrected exchange isotherm models (left: Ba-K-Y, right: Ca-K-Y)

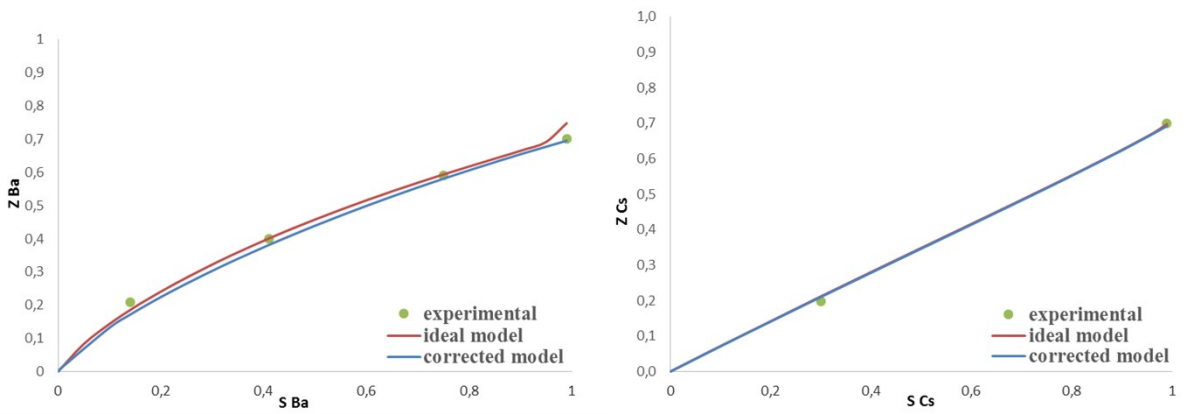

Figure S4. Comparison between ideal and corrected exchange isotherm models (left: Ba-Ca-Y, right: Cs-K-Y)

Table S1. Localization of exchanged cations in faujasite X[i]

Zeolite	site I	site I'	site II'	site II	site III	site III'	Not characterized
$Na_{86}X$	0	32	0	32	0	22	
$K_{92}Al_{92}Si_{100}O_{384}$	15.3	12.5		29.9	21.2	8.6	4
$Cs_{46}Na_{38}X$	0Cs 15Na	2Cs 15Na	15Cs	3Cs	26Cs 7Na	0	0
$Ba_{43}Na_3X$	1Ba	15.8Ba 1Na	0	29.5Ba	0	0	0
$Ca_{41}Na_3X$	12.6Ca	4Ca	0	26Ca	0	0	0

Table S2. Localization of exchanged cations in faujasite Y[i]

Zeolite	site I	site I'	site II'	site II	Site III	Not characterized
$Na_{52}Y$	4	16		32		
$K_{57}Y$	12	14		30		1
$Cs_{37.3}Na_{16}Y$	12Na	6Cs 4Na	7Cs	19Cs	5Cs	
$Ba_{23}Na_6Y$	7Ba	4.7Ba		11.4Ba 3.7Na		
$Ca_{26.8}Na_{3.4}Y$	8.3Ca	5.8Ca		16.3Ca		

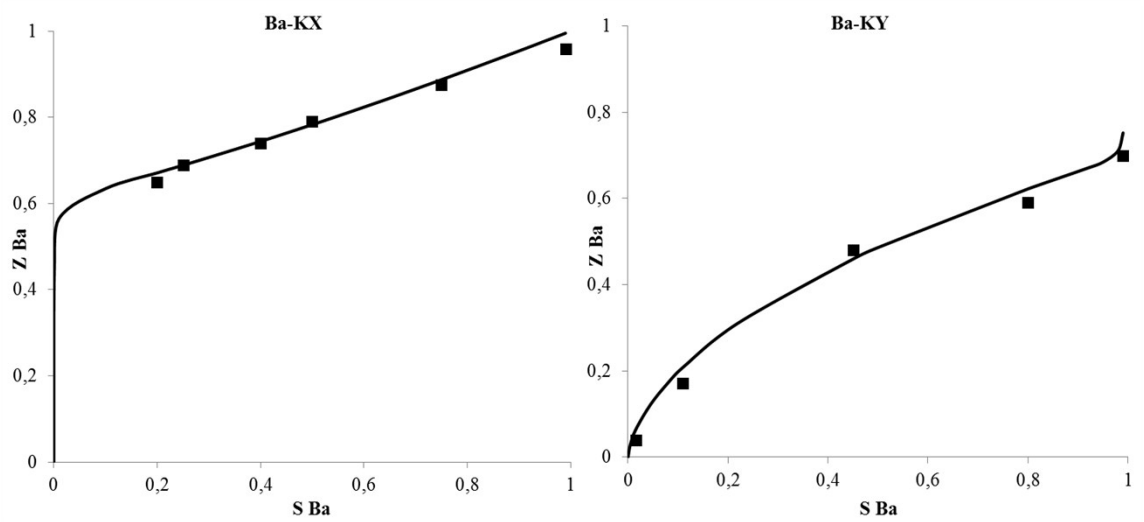

Figure S5. Isotherms for (a) BaKX and (b) BaKY, (■) Experimental data - (▬) model

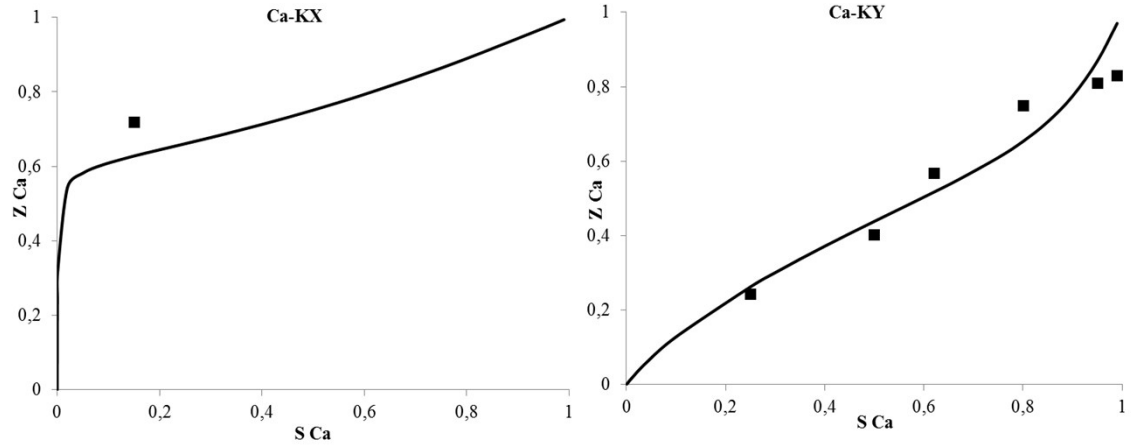

Figure S6. Isotherms for (a) CaKX and (b) CaKY, (■) Experimental data - (▬) model

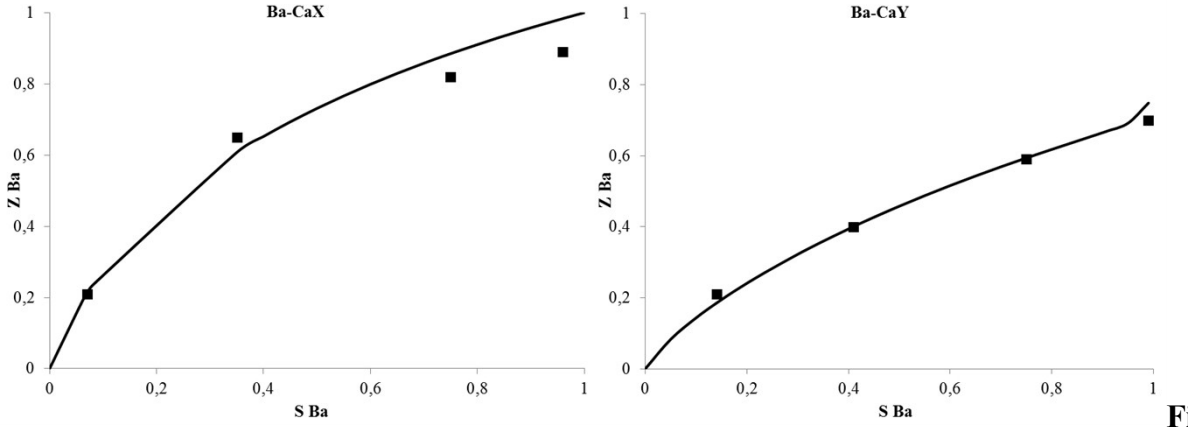

Figure S7. Isotherms for (a) BaCaX and (b) BaCaY, (■) Experimental data - (▬) model

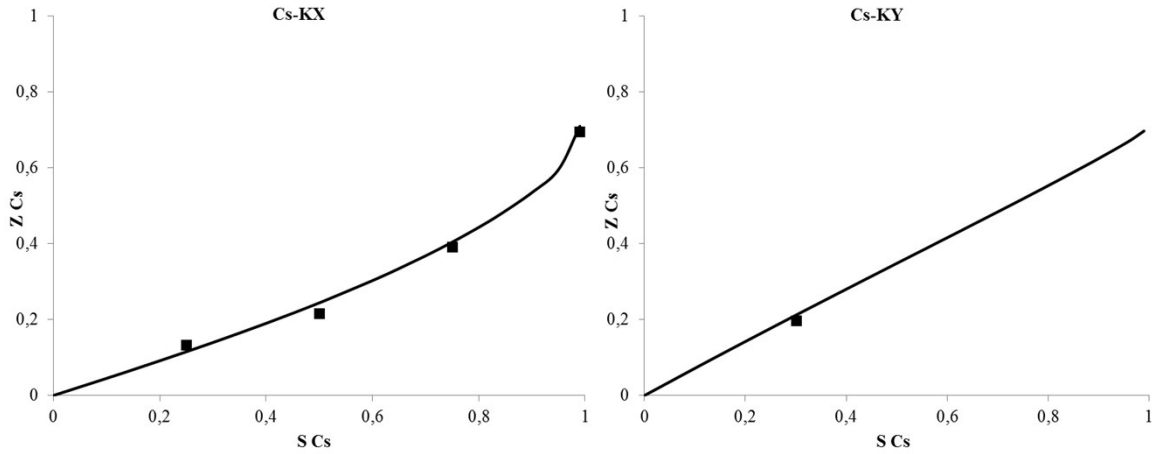

Figure S8. Isotherms for (a) CsKX and (b) CsKY, (■) Experimental data - (▬) model

Table S3. Mean Squared Error of the proposed isotherms models

	Mean Squared Error (MSE)	
System	FAU X	FAU Y
Cs/Na	0,00131462	0,000170089
K/Na	0,00076546	0,000726114
Ca/Na	0,00250738	0,000945906
Ba/Na	0,00083485	0,00108128
Cs/K	0,00036024	9,95915E-05
Ca/K	0,00846931	0,006125392
Ba/K	0,00478452	0,001244386
Ba/Ca	0,0036985	0,000743493

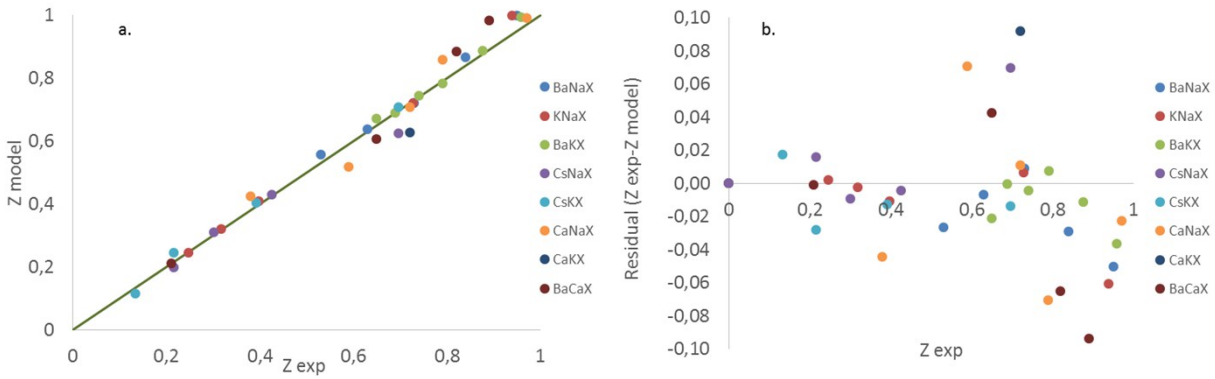

Figure S9. a. Parity plot, b. Residual plot for X-exchanged FAU models

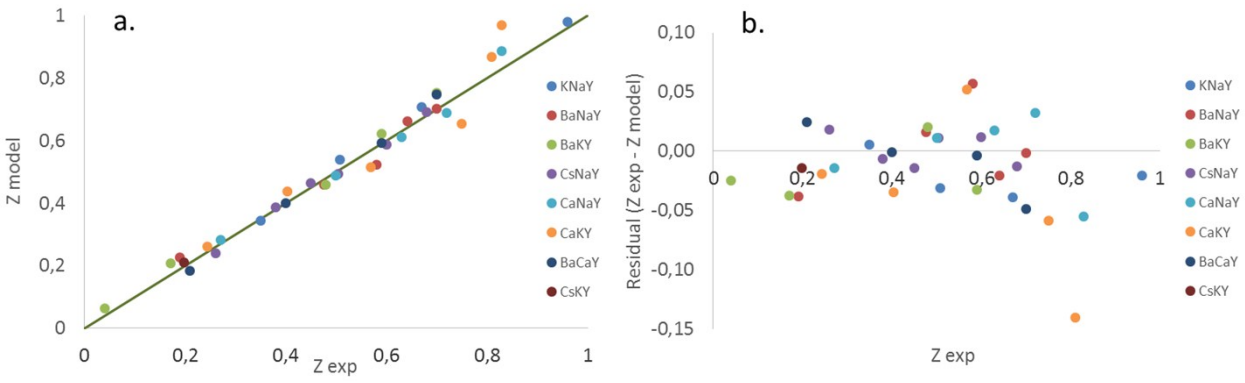

Figure S10. a. Parity plot, b. Residual plot for Y-exchanged FAU models

Table S4. Standard Deviation σ of the proposed isotherms models

	Standard Deviation $\sigma = \sqrt{MSE}$	
System	FAU X	FAU Y
Cs/Na	0,03625771	0,013041829
K/Na	0,02766686	0,026946494
Ca/Na	0,05007372	0,03075559
Ba/Na	0,02889378	0,032882829
Cs/K	0,01897993	0,009979556
Ca/K	0,09202886	0,078264882
Ba/K	0,06917024	0,035275853
Ba/Ca	0,06081529	0,027267065

Table S5. Deduced selectivity coefficients for Ca/Cs and Ba/Cs systems

		FAU X		
	j	**① site I,I'**	**② site II,II',III**	**③ site III,III',II**
	p_j	0.37	0.37	0.26
		deduced coefficients		
1	Kj Ca/Cs	2^E8	2.75	1138
2	Kj Ba/Cs	1^E9	4.29	2466
		FAU Y		
	j	**① site I'**	**② site I**	**③ site II**
	p_j	0.3	0.08	0.62
3	K_j Ca/Cs	4^E5	67	1.4
4	K_j Ba/Cs	0	967	2.31

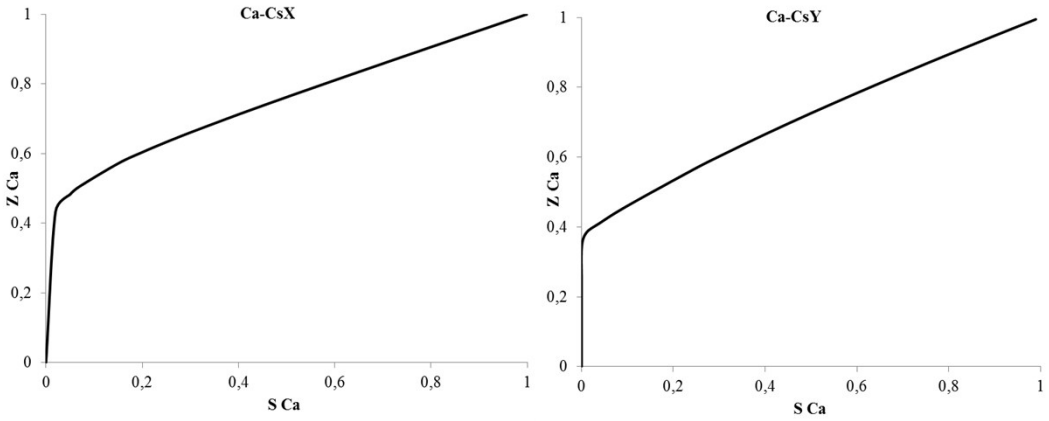

Figure S11. Isotherms for (a) CaCsX and (b) CaCsY

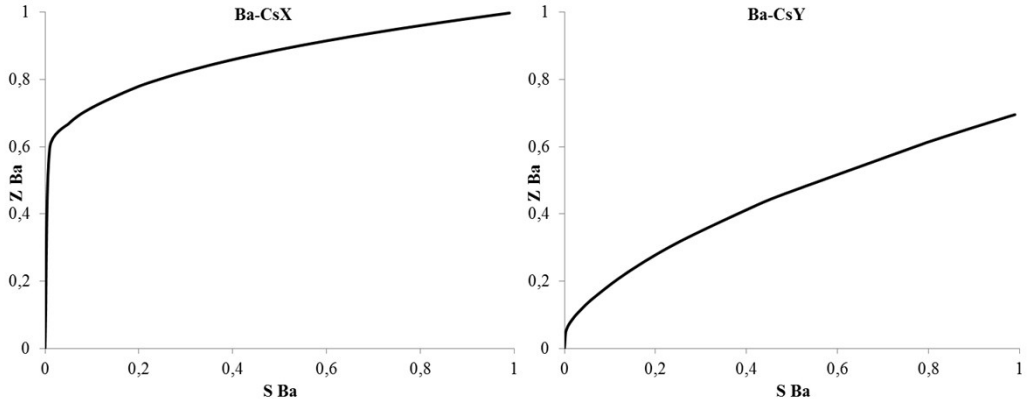

Figure S12. Isotherms for (a) BaCsX and (b) BaCsY

Table S6. Predicted cationic distribution of all exchanged faujasites studied. Number of cations per site group for a unit cell

Exchanged faujasite	S I,I'	SII	SIII
NaX (100-0)	31.8	31.8	22.4
NaY (100-0)	19.8	32	0.0
NaKX (68-32)	30.6 Na 1.3 K	21.2 Na 10.6 K	6.6 Na 15.8 K
NaKX (27-73)	19.5 Na 12.3 K	3.7 Na 28.1 K	0.6 Na 21.8 K
KX (6-94)	4.8 Na 27 K	0.5 Na 31.4 K	0.1 Na 22 K
NaKY (65-35)	18.5 Na 1.3 K	15.7 Na 16.5 K	n.a
NaKY (33-67)	13.1 Na 6.7 K	3.7 Na 28.6 K	n.a
KY (4-96)	1.8 Na 18 K	0.2 Na 32 K	n.a
NaCsY (74-26)	19.8 Na	18.9 Na 13.4 Cs	n.a
NaCsX (82-18)	31.8 Na	29.0 Na	9.3 Na

		2.9 Cs	13.1 Cs
NaCsX (51-49)	31.8 Na	10.7 Na 21.2 Cs	0.8 Na 21.6 Cs
NaCsX (43-57)	31.7 Na	4.2 Na 27.7 Cs	0.2 Na 22.1 Cs
NaCsY (62-38)	19.8 Na	11.5 Na 20.8 Cs	n.a
NaCsY (55-45)	19.7 Na	7.8 Na 24.5 Na	n.a
NaCsY (32-68)	18.3 Na 1.4 Cs	0.1 Na 32 Cs	n.a
NaCsY (32-68)	18.3 Na 1.4 Cs	0.1 Na 32 Cs	n.a
CsKX (25-75)	0.1 Cs 31.7 K	9.2 Cs 22.6 K	12.3 Cs 10.1 K
CsKX (48-52)	0.6 Cs 31.3 K	21.4 Cs 10.4 K	19.2 Cs 3.1 K
CsKY (20-76)	0.5 Cs 17.2 K	10.2 Cs 22.1 K	n.a
CsKY (43-57)	1.5 Cs 18.3 K	21.2 Cs 11.1 K	n.a
NaCaX (41-59)	8.3 Na 11.7 Ca	26.2 Na 13.9 Ca	n.a
NaCaX (32-68)	5.5 Na 13.2 Ca	21.8 Na 16.2 Ca	0.1 Na
NaCaX (28-72)	4.5 Na 13.6 Ca	19.5 Na 17.3 Ca	0.1 Na
CaX (3-97)	0.3 Na 15.7 Ca	2.2 Na 26 Ca	n.a
NaCaY (73-27)	19.5 Na	18.4 Na 6.9 Ca	n.a
NaCaY (50-50)	18.3 Na 0.7 Ca	7.3 Na 12.5 Ca	n.a
CaY (17-83)	8.2 Na 5.8 Ca	0.1 Na 16.1 Ca	n.a
NaBaX (49-51)	14.5 Na 10.8 Ba	26.6 Na 11.5 Ba	n.a
NaBaX (27-73)	2.7 Na 14.8 Ba	20.0 Na 16.9 Ba	n.a
BaX (5-95)	0.3 Na 15.8 Ba	3.9 Na 25.1 Ba	n.a
NaBaY (81-19)	19.1 Na	23.0 Na 4.6 Ba	n.a
NaBaY (52-48)	17.6 Na 1.1 Ba	10.8 Na 10.7 Ba	n.a
NaBaY (42-58)	16.6 Na 1.6 Ba	5.1 Na 13.6 Ba	n.a
NaBaY (36-64)	16.1 Na 1.8 Ba	2.5 Na 14.9 Ba	n.a

NaBaY (30-70)	15.5 Na 2.1 Ba	0.1 Na 16.1 Ba	n.a
CaKX (62-37)	15.2 Ca 1.4 K	11.8 Ca 25.4 K	5.2 K
CaKX (72-27)	15.6 Ca 0.5 K	15.6 Ca 20.4 K	2.5 K
CaKY (24-72)	1.2 Ca 15.3 K	5.2 Ca 21.8 K	
CaKY (40-52)	1.7 Ca 12.2 K	8.9 Ca 14.5 K	
CaKY (57-40)	2.5 Ca 13.2 K	12.4 Ca 7.5 K	
BaKX (16-80)	5.7 Ba 17 K	1.3 Ba 28.9 K	22.7 K
BaKX (76-22)	15.8 Ba	17.1 Ba 15.6 K	4.4 K
BaKX (65-31)	15.7 Ba	12.5 Ba 20.8 K	8.4 K
BaKX (87-12)	15.9 Ba	21.6 Ba 10.9 K	
BaKX (74-22)	15.8 Ba	16.3 Ba 16.5 K	5.2 K
BaKX (92.5-7.5)	15.9 Ba	23.8 Ba 6.5 K	
BaKX (98-2)	15.9 Ba	26.3 Ba 1.6 K	
BaKY (4-93)	1 Ba 16.1 K	0.7 Ba 30.9 K	
BaKY (17-79)	1.6 Ba 14.6 K	2.9 Ba 26.4 K	
BaKY (48-48)	2.0 Ba 13.8 K	10.7 Ba 10.8 K	
BaCsX (81-14)	15.9 Ba	19.2 Ba 10.8 Cs	
BaCsX (90-7)	15.9 Ba	22.9 Ba 5.5 Cs	
BaCsX (88-10)	15.9 Ba	22.4 Ba 7.4 Cs	
BaCsY (20-50)	1.9 Ba	3.5 Ba 25.2 Cs	
BaCsY (43-27)	2.0 Ba	9.3 Ba 13.6 Cs	
BaCaX (21-76)	5.8 Ba 8.8 Ca	3.2 Ba 23.8 Ca	
BaCaX (45-52)	10.7 Ba 4 Ca	8.8 Ba 18.3 Ca	
BaCaX (89-6)	13.8 Ba	23.0 Ba 4.1 Ca	
BaCaX (68-30)	15.1 Ba	15.8 Ba	

		11.3 Ca
BaCaY (21-71)	1.6 Ba 6.2 Ca	4.0 Ba 12.1 Ca
BaCaY (40-41)	1.9 Ba 3 Ca	8.5 Ba 7.6 Ca

[i] T. Frising, P. Leflaive, *Microporous Mesoporous Materials,* 2008, **114**, 27.