Supplemental information:

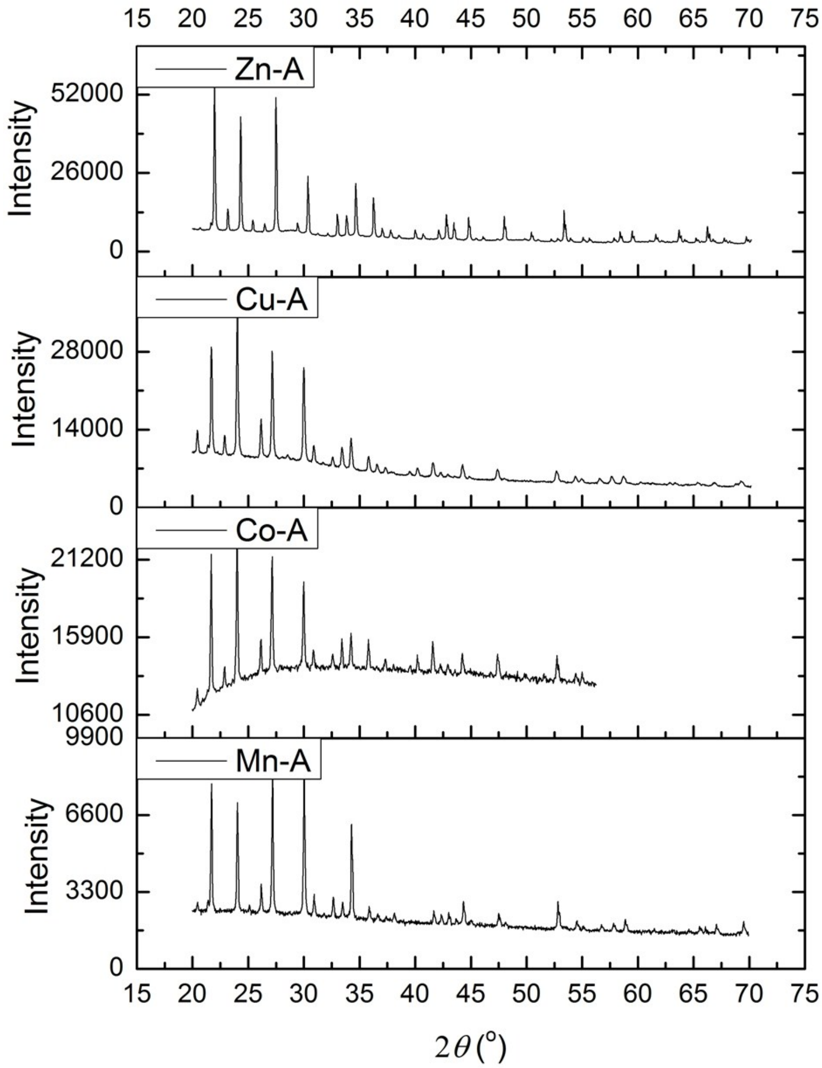

Figure 1 XRD patterns of transition metal ion exchanged zeolite A, sample XRD patterns match with previously reported data [14-17].

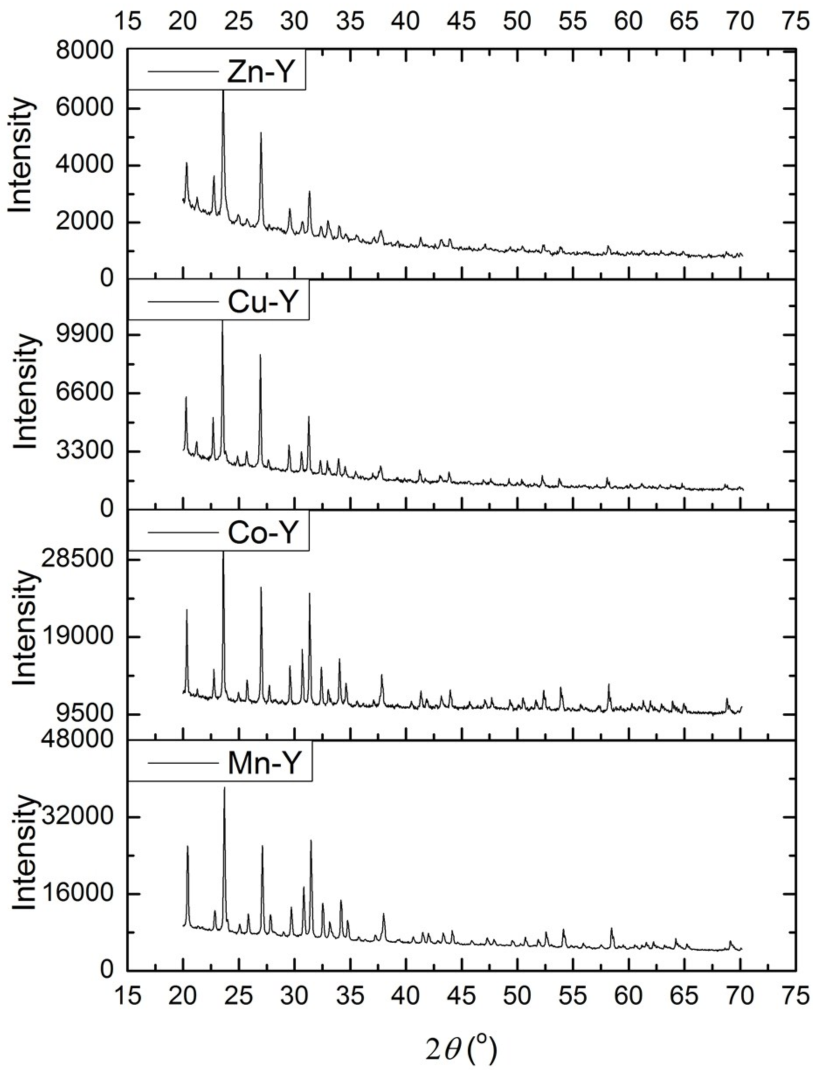

Figure 2 XRD patterns of transition metal ion exchanged zeolite Y, sample XRD patterns match with previously reported data [18-21].

Table 1. Thermochemical cycle for calculation of enthalpy of formation from oxides ($\Delta H_{f,ox}$) for hydrated transition metal exchanged zeolite A and Y

Reactions	Enthalpy
$xNa_2O(s,25°C)+yMO(s,25°C)+iAl_2O_3(s,25°C)+jSiO_2(s, 25°C)$ $+qH_2O(s, 25°C)\rightarrow Na_xM_yAl_iSi_jO_2 (H_2O)_q(s, 25°C)$	$\Delta H_{f,ox}(M)$
$Na_2O(s,25°C) \rightarrow Na_2O(soln, 700°C)$	ΔH_1
$MO(s,25°C) \rightarrow MO(soln, 700°C)$	ΔH_2
$Al_2O_3(s, 25°C) \rightarrow Al_2O_3(soln, 700°C)$	ΔH_3
$SiO_2(s, 25°C) \rightarrow SiO_2(soln, 700°C)$	ΔH_4
$H_2O(s, 25°C) \rightarrow H_2O(g, 700°C)$	ΔH_5
$Na_xM_yAl_iSi_jO_2(s, 25°C) \rightarrow Na_xM_yAl_iSi_jO_2(soln, 700°C)$	ΔH_6
$\Delta H_{f,ox}(M)=(x/2)\Delta H_1+y\Delta H_2+(i/2)\Delta H_3+j\Delta H_4+q\Delta H_5-\Delta H_6$	

Table 2. Drop Solution Enthalpies for Constituent Oxides in Lead Borate at 700 ˚C and Formation Enthalpies from Elements at 25 ˚C for Oxides and Ions in Aqueous Solution .

Material	Formula	ΔH_{ds}(kJ mol^{-1})	$\Delta H_{f,el}$(kJ mol^{-1})
Quartz	SiO_2	39.13±0.32[a]	-910.70±1.00[b]
α-Alumina	Al_2O_3	107.93±0.98[a]	-1675.70±1.30[b]
Water	H_2O	68.98±0.10[a]	-285.08±0.10[b]
Sodium Oxide	Na_2O	-113.10±0.83[a]	-414.84±0.25[b]
Manganese Oxide	MnO	43.1±0.8[c]	-385.22±0.46[b]
Cobalt Oxide	CoO	57.23±0.84[d]	-237.94±1.26[b]
Copper Oxide	CuO	67.9±0.6[e]	-157.32±1.26[b]
Zinc Oxide	ZnO	51.98±0.88[d]	-35.05±0.27[b]
Sodium ion	Na^+(aq, M=1)	-	-240.30±0.06[b]
Manganese ion	Mn^{2+}(aq, M=1)	-	-220.70±0.12[b]
Cobalt ion	Co^{2+}(aq, M=1)	-	-58.20±0.50[b]
Copper ion	Cu^{2+}(aq, M=1)	-	64.77±0.10[b]
Zinc ion	Zn^{2+}(aq, M=1)	-	-153.39±0.20[b]

[a] I. Kiseleva, A. Navrotsky, I.A. Belitsky and B.A. Fursenko, *American Mineralogist*, 1996, **81**, 658-667.

[b] R. A. Robie, B. S. Hemingway, u.s. geological survey bullet in 1452, 1995.

[c] S. Fritsch and A. Navrotsky, *Journal of the American Ceramic Society*, 1996, **79**, 1761-1768.

[d] R. k. Allada, E. Peltier, A. Navrotsky, W. H. Casey, C. A. Johnson, H. T. Berbeco and D. L. Sparks, *Clays and Clay Minerals*, 2006, **54**, 409-417.

[e] Z. Zhou and A. Navrotsky, *Journal of Materials Research*, 1992, **7**, 2920-2935.

Table 3. Thermochemical cycle for calculation of enthalpy of formation from elements ($\Delta H_{f,el}$) at 25°C for transition metal exchanged zeolite A and Y

Reactions	Enthalpy
xNa_2O(s,25°C)+yMO(s,25°C)+iAl_2O_3(s,25°C)+$jSiO_2$(s, 25°C)+qH_2O(s, 25°C)→$Na_xM_yAl_iSi_jO_2(H_2O)_q$(s, 25°C)	$\Delta H_{f,ox}(M)$
Elements →Na_2O(s,25°C)	ΔH°_1
Elements →MO(s,25°C)	ΔH°_2
Elements →Al_2O_3(s, 25°C)	ΔH°_3
Elements →SiO_2(s, 25°C)	ΔH°_4
Elements →H_2O(s, 25°C)	ΔH°_5
Elements→$Na_xM_yAl_iSi_jO_2$(s, 25°C)	ΔH°_6
$\Delta H_{f,el}$(M-zeolite)=$(x/2)\Delta H^{\circ}_1+y\Delta H^{\circ}_2+(i/2)\Delta H^{\circ}_3+j\Delta H^{\circ}_4+q\Delta H^{\circ}_5+\Delta H^{\circ}_6$	

Calculation of enthalpies of exchange ΔH_{ex}:

Step 1: Generalize the compositions of M-zeolite according to Na-zeolite A and Y, the metal content is calculated by use exchange percentage, for example:
For Mn-zeolite A: Na=0.481×(1-0.999)=0.0005; Mn=0.481×0.999/2=0.2403.

Table 4. The generalized compositions of M-zeolites

Ratio	2M/(2M+Na)	Na	M	Al	Si	O
Na-A		0.481		0.492	0.510	2
Mn-A	0.999	0.0005	0.240	0.492	0.510	2
Co-A	0.996	0.0019	0.239	0.492	0.510	2
Cu-A	0.980	0.0096	0.236	0.492	0.510	2
Zn-A	0.998	0.0010	0.240	0.492	0.510	2
Na-Y		0.276		0.284	0.716	2
Mn-Y	0.972	0.008	0.134	0.284	0.716	2
Co-Y	0.846	0.043	0.117	0.284	0.716	2
Cu-Y	0.963	0.010	0.133	0.284	0.716	2
Zn-Y	0.973	0.007	0.134	0.284	0.716	2

Step 2: The corresponding drop solution enthalpies are listed in first column (S.I. Table 5). According to the composition in Step 1, calculate the drop solution enthalpies of anhydrous M-zeolite by Na correction.

$$\Delta H_{ds}(\text{M-zeolite})=\{\Delta H_{ds}(\text{Na, M-zeolite})-x\Delta H_{ds}(\text{Na-zeolite})\}/y \qquad (1)$$

Then, calculate the enthalpies of formation from oxides for anhydrous M-zeolite $\Delta H_{f.ox}(M)$ by using equation (2):

$$\mathbf{\Delta H_{f,ox}}(\text{M-zeolite}) = \sum_{i=1}^{5} \Delta H_{ds}(oxides) - \Delta H_{ds}(M\text{-}zeolite)$$

$$=(x/2)\mathbf{\Delta H_{ds}}(Na_2O)+y\mathbf{\Delta H_{ds}}(MO)+(i/2)\mathbf{\Delta H_{ds}}(Al_2O_3)+j\mathbf{\Delta H_{ds}}(SiO_2) + q\mathbf{\Delta H_{ds}}(H_2O)-\mathbf{\Delta H_{ds}}(\text{M-zeolite}) \qquad (2)$$

Table 5. Drop solution enthalpies before and after Na correction, formation enthalpies from oxides for pure M-zeolites.

	ΔH_{ds}(hy) (kJ mol^{-1})	**ΔH_{ds}(dhy) (kJ mol^{-1})**	**ΔH_{ds}(pure) (kJ mol^{-1})**	**$\Delta H_{f.ox}$(pure) (kJ mol^{-1})**
Mn-A	131.00(8) ±1.00	34.47±0.99	34.42±0.99	22.47±1.15
Co-A	110.65(9) ±1.67	10.04±1.66	9.76±1.66	50.65±1.71
Cu-A	104.20(8) ±5.14	10.43±5.11	9.04±5.14	54.76±5.15
Zn-A	123.26(8) ±1.30	41.59±1.30	41.48±1.30	17.58±1.36
Mn-Y	126.71(8) ±1.81	41.27±1.79	41.21±1.81	11.72±1.98
Co-Y	148.66(8) ±2.15	35.23±2.07	34.62±2.15	23.41±2.19
Cu-Y	135.56(8) ±1.70	23.05±1.68	22.78±1.70	34.12±1.74
Zn-Y	136.56(8) ±1.71	41.62±1.70	41.56±1.71	12.68±1.75

ΔH_{ds}(hy)- drop solution enthalpies for hydrous M-zeolites;
ΔH_{ds}(dhy)- drop solution enthalpies for anhydrous M-zeolites;
ΔH_{ds}(pure)- Na corrected drop solution enthalpies for anhydrous M-zeolites;
$\Delta H_{f.ox}$(pure)- formation enthalpies from oxides for Na corrected anhydrous M-zeolites.

Step 3: Calculate the formation enthalpies from elements by using equation (3), the $H_{f,ox}$(M-zeolite) is from $\Delta H_{f.ox}$(pure) in Table 5.

$$\mathbf{\Delta H_{f,el}}\text{(M-zeolite)}=\sum_{i=1}^{5}\Delta H^{o}_{f,el}(oxides)+\Delta H_{f,ox}\,(M\text{–}zeolite)$$

$$=(x/2)\mathbf{\Delta H^{\circ}_{f,el}}(Na_2O,s)+y\mathbf{\Delta H^{\circ}}_{f,el}(MO,s)+(i/2)\mathbf{\Delta H^{\circ}}_{f,el}(Al_2O_3,s)+j\mathbf{\Delta H^{\circ}}_{f,el}(SiO_2,s)+\mathbf{\Delta H_{f,ox}}\text{(M-zeolite)} \qquad (3)$$

Table 6. Formation enthalpies from elements for M-zeolite.

	$\Delta H_{f,el}$(dhy) (kJ mol^{-1})
Mn-A	-947.49±1.31
Co-A	-883.81±1.87
Cu-A	-860.28±5.50
Zn-A	-867.99±1.52
Mn-Y	-931.45±2.12
Co-Y	-899.43±2.21
Cu-Y	-877.60±1.92
Zn-Y	-882.17±1.90

Step 4: Calculate the enthalpies of exchange by using equation (4):

$$\mathbf{\Delta H}_{ex} = \Delta H_{f,el}\text{(M-zeolite)}+x\ \Delta H_{f,el}\ (Na^{+})-\ \Delta H_{f,el}\text{(Na-zeolite)}-\ (x/2)\Delta H_{f,el}(M^{2+}) \qquad (4)$$

Table 7. List of enthalpies of exchange for M-zeolite.

	ΔH_{ex}(kJ mol^{-1})
Mn-A	32.24±1.78
Co-A	56.76±2.22
Cu-A	50.66±5.63
Zn-A	95.52±1.94
Mn-Y	3.83±2.40
Co-Y	10.86±2.48
Cu-Y	15.72±2.23
Zn-Y	41.26±2.22