Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Exploring the adsorption of short and long chain per- and polyfluoroalkyl substances (PFAS) to different zeolites using environmental samples

Maura Mancinelli[a,*], Annalisa Martucci[a], Lutz Ahrens[b,*]

[a] Department of Physics and Earth Science, University of Ferrara, via Saragat, 1, 44122 Ferrara, Italy

[b] Department of Aquatic Sciences and Assessment, Swedish University of Agricultural Sciences (SLU), P.O. Box 7050, SE-750 07 Uppsala, Sweden

e-mail addresses: *maura.mancinelli@unife.it (M. Mancinelli), *lutz.ahrens@slu.se (L. Ahrens).

Supplementary Information

Table SI.1. Details of all investigated zeolites.

Sample	Framework-type	Supplier and product code	SiO_2/Al_2O_3 mole ratio	Surface Area (BET, m^2/g)	Nominal cation form
BETA25	BEA	Zeolyst International CP814E*	25	680	Ammonium
BETA360	BEA	Zeolyst International CP811C*300	300	620	Hydrogen
Y720	FAU	Zeolyst International CBV720	30	780	Hydrogen
Y760	FAU	Zeolyst International CBV760	60	720	Hydrogen
Y390	FAU	Tosoh Corporation HSZ390HUA	500	630	Hydrogen
MOR	MOR	Tosoh Corporation 690HUA	240	450	Hydrogen
L	LTL	Tosoh Corporation 500KOA	6.1	290	Potassium
CHA	CHA	Natural Chabasite (65%wt. Chabasite) from Zeolite Italia			

Table SI.2 $\sum$PFAS uptake (%) from RW-F after 24h contact time.

	PFAS uptake (%)
RW1-F	
Beta25-RW1-F	97.7
BETA360-RW1-F	97.2
MOR-RW1-F	96.5
Y760-RW1-F	94.8
CHA-RW1-F	75.1
PAC-RW1-F	99.9
RW2-F	
Beta25-RW2-F	99.3
Beta360-RW2-F	98.3
MOR-RW2-F	97.6
Y760-RW2-F	96.0
CHA-RW2-F	76.2
PAC-RW2-F	99.9
Beta25-RW3A-F	99.2
Beta360-RW3A-F	97.8
MOR-RW3A-F	97.2
Y760-RW3A-F	94.9
CHA-RW3A-F	53.2
PAC-RW3A-F	99.9
RW3B-F	
Beta25-RW3B-F	99.3
Beta360-RW3B-F	96.6
MOR-RW3B-F	97.0
Y760-RW3B-F	96.4
CHA-RW3B-F	81.3
PAC-RW3B-F	99.9

Table SI.3 Unit-cell parameters and Crystallite size (Å) for (A) Beta360, (B) CHA, (C) MOR, (D) Y760, (E) Y390, (F) AgY760, (G) AgY390 zeolites, before and after PFAS loading and thermal treatments up to 1400°C. Crystallite size obtained from the Scherrer equation. Legend: AS: as-synthetized, bare sample; 18PFAS: loaded with ∑PFAS solution and data collected on the sample subjected to 24 h contact time; REG air: samples heated up to 1400°C after ∑PFAS uptake; RW-F series: loaded towards RW-F and data collected on the sample subjected to 24 h contact time.

A.

BEA-type		**Beta360**	**Beta360-18PFAS**	**REG_air_Beta360-18PFAS**	**Beta360-RW1-F**	**Beta360-RW2-F**	**Beta360-RW3A-F**	**Beta360-RW3B-F**
Polytype A *P*4122	**a = b (Å)**	11.148(6)	11.087(1)	11.125(2)	11.064(2)	11.042(5)	11.199(2)	11.076(3)
	c (Å)	23.290(8)	23.425(3)	23.420(5)	23.274(4)	23.607(1)	23.271(7)	23.419(6)
	α = β = γ (°)	90	90	90	90	90	90	90
	V (Å^3)	2894.2(9)	2879.7(2)	2898.7(1)	2849.4(1)	2878.7(8)	2918.5(2)	2873.4(3)
Polytype B *C*2/*c*	**a (Å)**	17.843(3)	17.657(2)	17.747(1)	17.639(4)	17.621(5)	17.649(6)	17.548(4)
	b (Å)	18.242(1)	18.609(7)	18.970(7)	18.580(6)	18.442(6)	18.508(1)	18.720(6)
	c (Å)	15.305(6)	15.420(3)	15.555(1)	15.473(1)	15.300(4)	15.318(5)	15.219(2)
	α = γ (°)	90	90	90	90	90	90	90
	β (°)	118.18(3)	117.30(2)	116.8(9)	116.94(9)	117.77(2)	116.65(2)	118.0(7)
	V (Å^3)	4390.8(3)	4502.1(2)	4673.4(8)	4520.8(5)	4399.0(2)	4471.5(6)	4414.1(3)
Crystallite size (Å)		80.3	82.9	80.2	83.4	82.9	85.1	80.2

B.

		CHA	**CHA-18PFAS**	**REG_air CHA-18PFAS**	**CHA-RW1 -F**	**CHA-RW2 -F**	**CHA-RW3A-F**	**CHA-RW3B -F**
***R*-3*m* Chabasite CHA-type**	**a = b (Å)**	13.7959(1)	13.7989(1)	-	13.7959(1)	13.7953(1)	13.7977(1)	13.8085(4)
	c (Å)	14.9716(2)	14.9768(2)	-	14.9685(2)	14.9711(2)	14.9738(2)	14.9840(5)
	V (Å^3)	2467.75(5)	2469.71(6)	-	2467.23(5)	2467.47(5)	2468.79(5)	2474.31(4)
	α = β (°)	90	90	-	90	90	90	90
	γ (°)	120	120	-	120	120	120	120
Crystallite size (Å)		974.5	1031.2	-	1041.6	1072.8	1153.8	1063.1

C.

		MOR	MOR-18PFAS	REG air MOR-18PFAS	MOR-RW1-F	MOR-RW2-F	MOR-RW3A-F	MOR-RW3B-F
Cmcm Mordenite (MOR)	a (Å)	18.0754(2)	18.0759(2)	18.0486(8)	18.0792(2)	18.0793(2)	18.0568(2)	18.0747(2)
	b (Å)	20.2380(2)	20.2419(2)	20.1151(7)	20.2457(2)	20.2504(2)	20.2321(2)	20.2432(2)
	c (Å)	7.46418(8)	7.46484(8)	7.4422(2)	7.46443(9)	7.46615(9)	7.46085(8)	7.46443(8)
	α=β= γ (°)	90	90	90	90	90	90	90
	V (Å^3)	2730.47(5)	2731.33(5)	2701.9(1)	2732.19(6)	2733.47(6)	2725.66(5)	2731.17(5)
Crystallite size (Å)		810.3	813.6	860.00	817.4	824.1	762.4	824.8

D.

		Y760	Y760-18PFAS	REG air Y760-18PFAS	Y760-RW1-F	Y760-RW2-F	Y760-RW3A-F	Y760-RW3B-F
Fd-3 FAU-type	a = b =c (Å)	24.2789(6)	24.2729(3)	24.2691(7)	24.2763(2)	24.2756(2)	24.2701(2)	24.2762(3)
	α=β= γ (°)	90	90	90	90	90	90	90
	V (Å^3)	14311.6(6)	14300.9(3)	14294.2(7)	14307.1(2)	14305.8(2)	14296.1(2)	14306.8(3)
Crystallite size (Å)		415.8	753.0	711.1	778.2	755.2	702.8	609.1

E.

		Y390	Y390-18PFAS
Fd-3*m* FAU-type	a = b =c (Å)	24.2882(4)	24.2845(1)
	α=β= γ (°)	90	90
	V (Å^3)	14328.1(4)	14321.6(1)
Crystallite size (Å)		669.3	642.7

F.

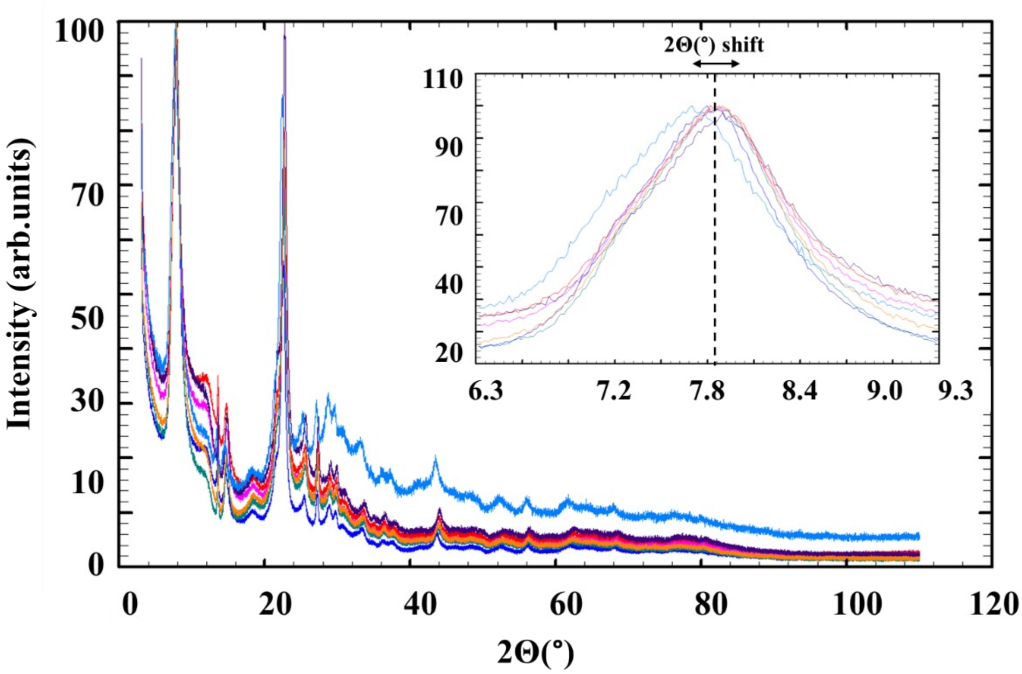
		AgY760	AgY760-18PFAS
Fd-3*m* FAU-type	a = b =c (Å)	24.2844(4)	24.2767(2)
	α=β= γ (°)	90	90
	V (Å^3)	14321.3(4)	14307.6(2)
Crystallite size (Å)		767.2	797.4

G.

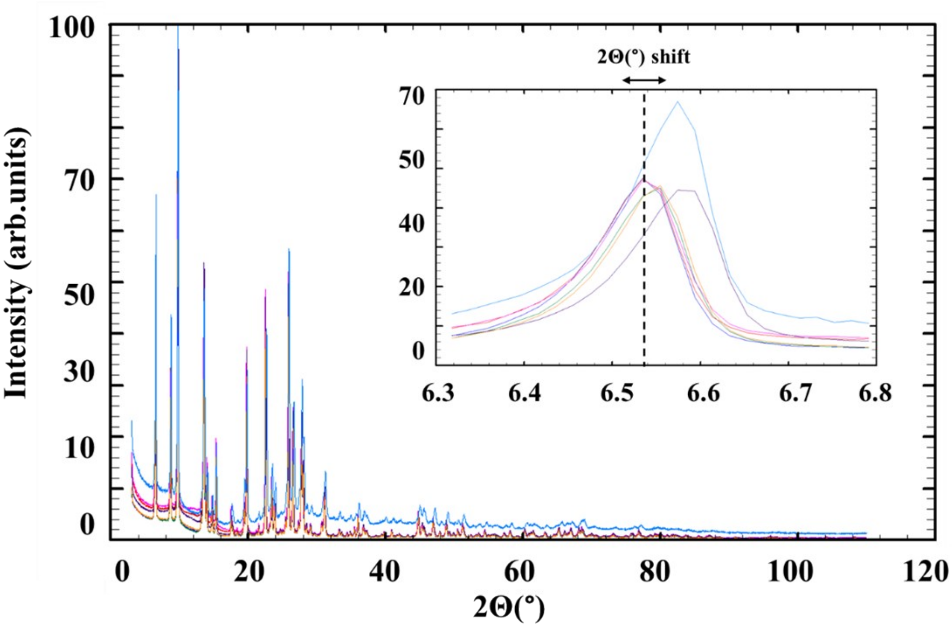
		AgY390	AgY390-18PFAS
Fd-3m FAU-type	a = b =c (Å)	24.2839(4)	24.2483 (1)
	α=β= γ (°)	90	90
	V (Å^3)	14320.5(4)	14257.5(4)
Crystallite size (Å)		651.9	637.1

Figure SI.1 X-ray powder diffraction pattern of (A) Beta360, (B) MOR, (C) CHA, (D) Y760, (E) Y390, (F) AgY760, (G) AgY390 zeolites. Colours legend: Blue line: as-synthetized sample; light blue line: sample heated at 900°C in air; green line: ∑PFAS-spiked with 24 h contact time; red line: RW1-F ∑PFAS-spiked with 24 h contact time; fuchsia: RW2-F ∑PFAS-spiked with 24 h contact time; violet line: RW3A-F ∑PFAS-spiked with 24 h contact time; orange line: RW3B-F ∑PFAS-spiked with 24 h contact time.

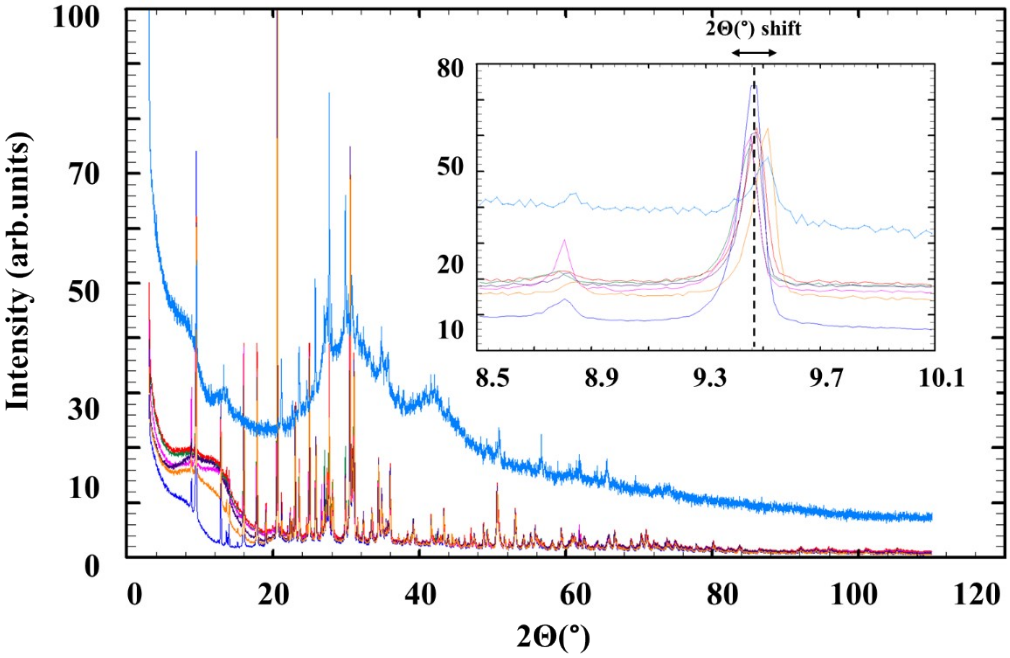
A. Beta360



B. MOR

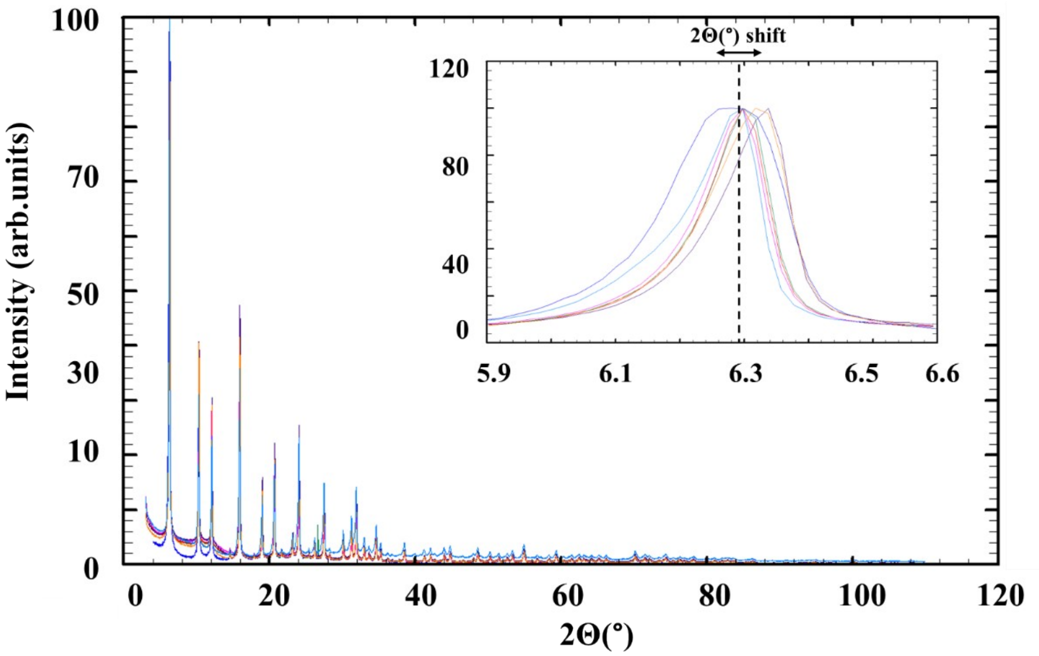


C. CHA



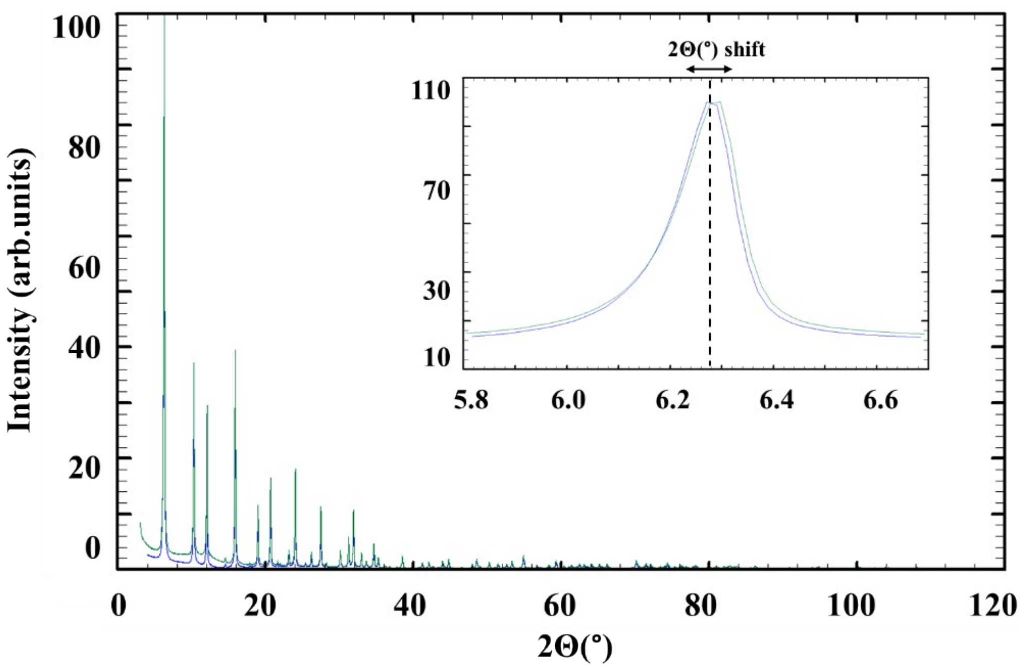
51

D. Y760

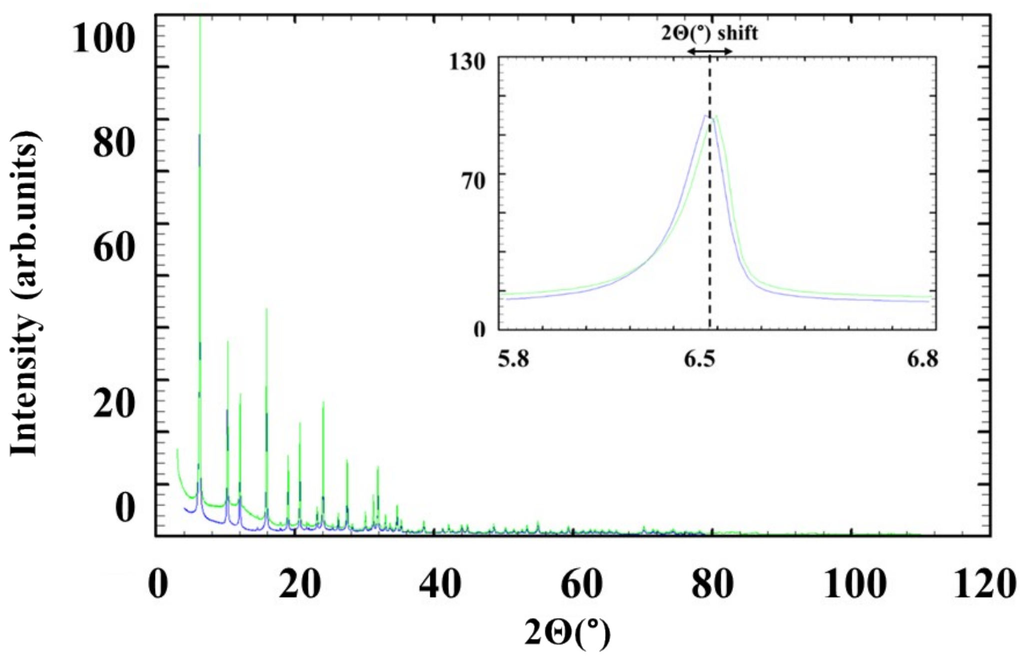


52

E. Y390



F. AgY760



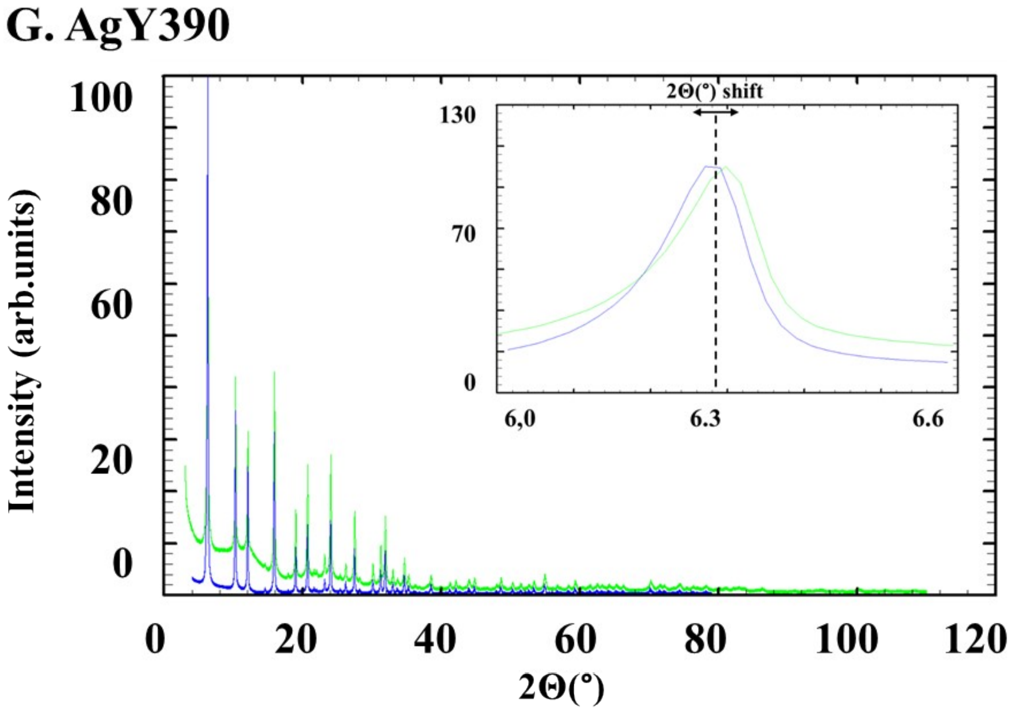
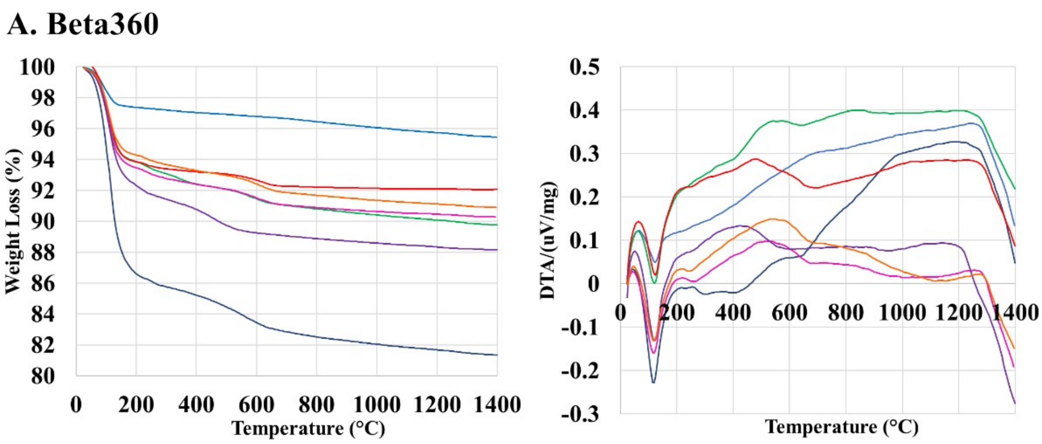
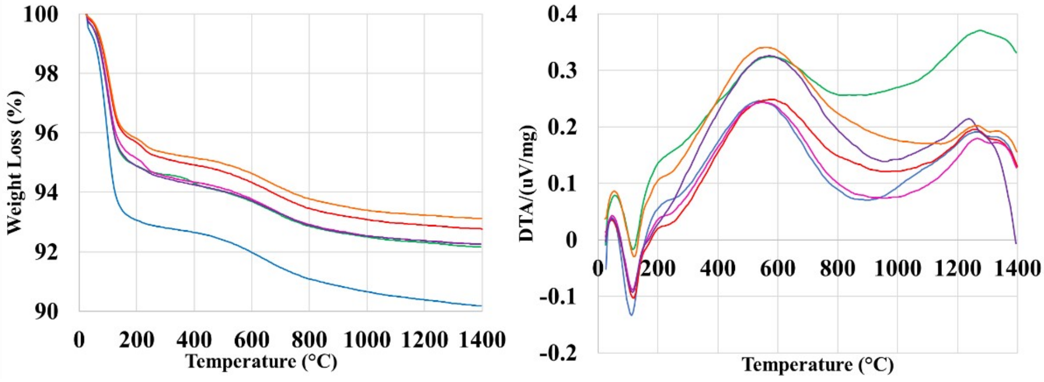


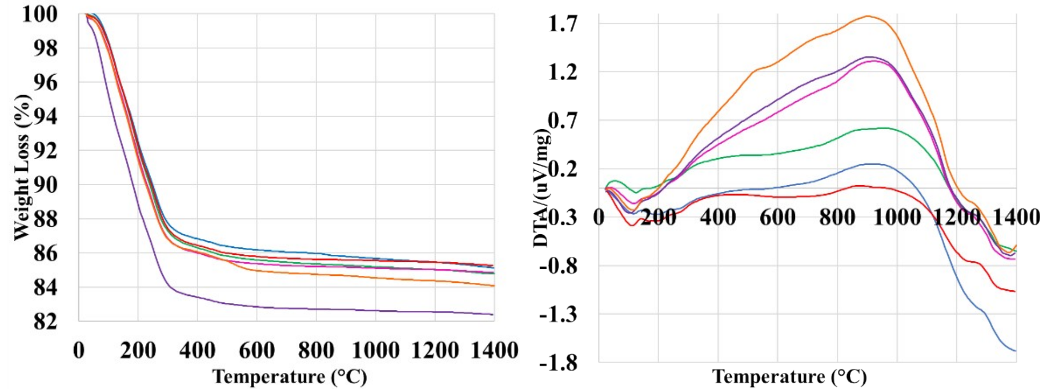
Figure SI.2 Thermogravimetric (TG) and differential thermal analysis (DTA) conducted in air controlled atmosphere from RT to 1400°C (10°C/min heating rate) of (A) Beta360, (B) MOR, (C) CHA, (D) Y760, (E) Y390, (F) AgY760, (G) AgY390 zeolites. Colours legend: Blue line: bare sample; light blue line: calcined bare sample; green line: ∑PFAS-spiked with 24 h contact time; red line: RW1-F ∑PFAS-spiked with 24 h contact time; fuchsia: RW2-F ∑PFAS-spiked with 24 h contact time; violet line: RW3A-F ∑PFAS-spiked with 24 h contact time; orange line: RW3B-F ∑PFAS-spiked with 24 h contact time.



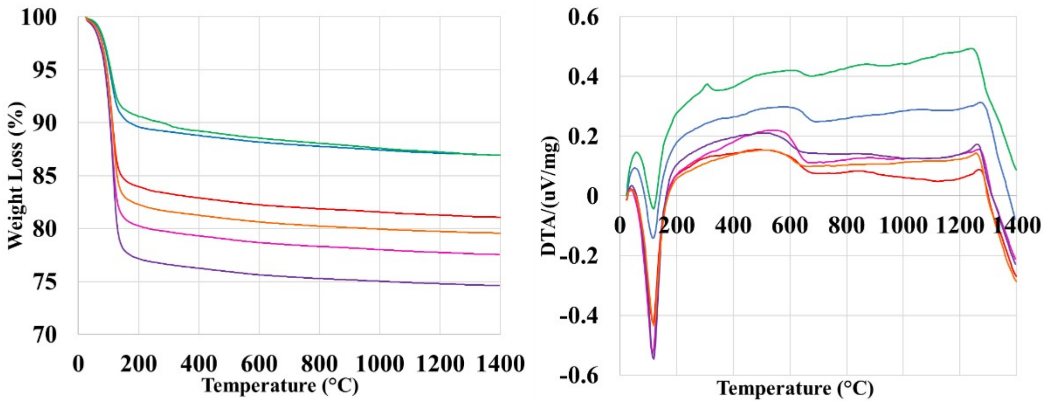
B. MOR



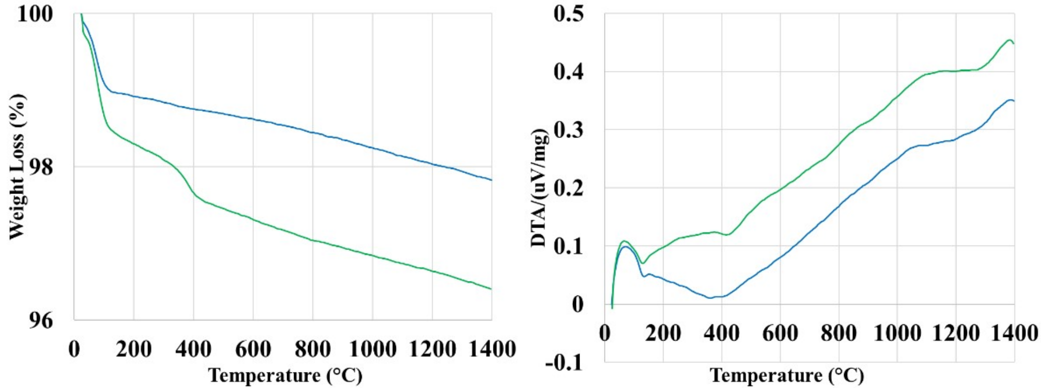
C. CHA



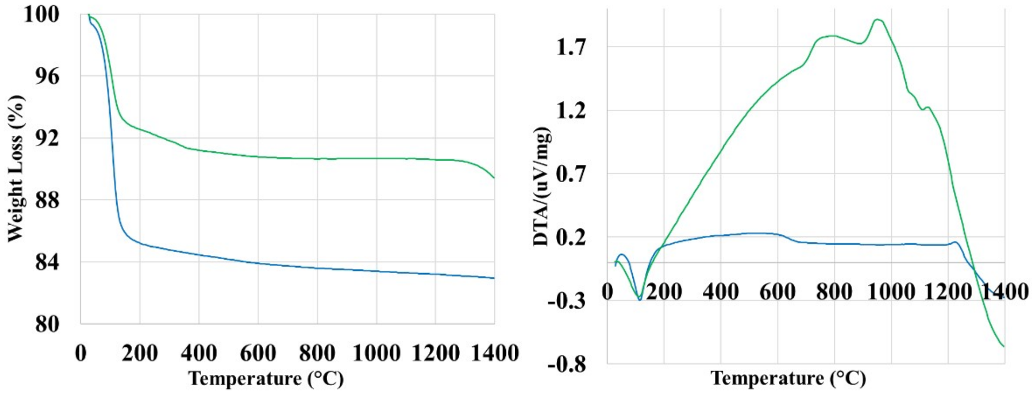
D. Y760



E. Y390



F. AgY760



G. AgY390