Supplementary Information

High temperature behaviour of Ag-exchanged Y zeolites used for PFAS sequestration from water.

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Tables SI1. Atomic bond distances for PFOA and PFOS molecules.

PFOS		PFOA	
Distance	Value(Å)	Distance	Value(Å)
C1-C1	2.35141(3)	C1-C1 [x2]	1.35731(2)
C1-C1	1.35759(1)	C2-C3	1.35728(2)
C1-C2	1.35759(2)	C2-C4	1.33862(2)
C1-C2	2.37314(3)	C2-C4	2.08664(3)
C1-C2	2.32818(3)	C3-C3	1.35697(2)
C1-C3	2.29788(3)	C3-C3	2.00820(3)
C1-C4	2.37624(3)	C3-O1n	2.26448(3)
C2-C3	1.35756(1)	C3-O1n	1.17228(2)
C2-C3	2.37292(3)	C3-O1n	2.08067(3)
C2-C5	2.27746(3)	C4-C5	1.31726(2)
C2-C4	1.33889(1)	C4-C4	1.37449(2)
C2-C4	2.32708(3)	C4-C4	1.71812(3)
C2-C4	2.08706(2)	C5-C4	1.31618(2)
C3-C3	1.35725(1)	C5-F1	1.25888(2)
C3-C3	2.00861(3)	C5-F1	1.26097(2)
C3-C3	2.33024(2)	C5-F2	1.15101(1)
C3-C4	2.33157(3)	F1-F2	2.07860(3)
C3-S	1.71387(2)	F1-F1	1.57379(2)
C3-S	1.38361(1)	F1-F1	2.48059(4)
C3-S	2.17486(2)	F1-F1	1.91742(2)
C3-S	1.67828(2)	O1n-H1	1.92601(3)
C4-C4	1.37477(1)	O1n-H1	1.92760(3)
C4-C4	1.71847(3)	O1n-H1	0.85697(1)
C4-C5	1.31753(1)	O1n-H1	0.85839(1)
C4-C5	2.36783(3)		
C5-C2	2.27596(3)		
C5-F1	2.45411(3)		
C5-F1	1.26123(2)		
F1-F1	1.57412(2)		
F1-F1	2.48109(4)		
F1-F1	1.91781(2)		
F1-F2	2.07902(3)		
F2-F1	2.07743(3)		
S-O1n	2.10599(2)		
S-O1n	1.35819(1)		
S-O1n	2.19509(3)		
S-O1n	1.40587(2)		
S-O2n	2.19071(3)		
S-O2n	1.57724(2)		
O1n-H1	2.02283(3)		
O1n-H1	1.56144(2)		

Tables SI2. Framework atomic coordinates, site occupancy, and atomic displacement parameters, ADPs (U_{iso}* = U_i/U_e*100 [Å^{-2}]) for the investigated AgY760 bare zeolite heated at 25, 200, 250, 550 and 900°C.

AgY760-25					
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0362(1)	0.3040(1)	0.1240(1)	0.9000	1.51
O1	0.0000	0.3555(1)	0.1444(1)	1.0000	1.61
O2	0.0033(1)	0.2533(1)	0.1088(1)	1.0000	1.61
O3	0.0779(1)	0.2860(1)	0.1720(1)	1.0000	1.61
O4	0.0702(1)	0.3221(1)	0.0702(1)	1.0000	1.61
Ag(I)	0.0000	0.0000	0.0000	0.0329	10.87
Ag(I')	0.0740	0.0740	0.0740	0.0715	10.87
Ag(IIb)	0.1889	0.1889	0.1889	0.0393	10.87
w1	0.4632	0.0886	0.0886	0.0830	2.58
w2	0.625	0.1249	0.3036	0.0832	1.47
w3	0.39800	0.24670	0.24670	0.0569	4.04
w4	0.2962	-0.0460	-0.0460	0.0639	5.32

AgY760-200					
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0361(1)	0.3042(1)	0.1240(1)	0.9000	1.30
O1	0.0000	0.3555(1)	0.1444(1)	1.0000	1.85
O2	-0.0034(1)	0.2534(1)	0.1091(2)	1.0000	1.85
O3	0.0782(1)	0.2862(2)	0.1717(1)	1.0000	1.85
O4	0.0700(1)	0.3221(1)	0.0700(1)	1.0000	1.85
Ag(I)	0.0000	0.0000	0.0000	0.0420	12.15
Ag(I')	0.0675(13)	0.0675(1)	0.0675(3)	0.0720	12.15
Ag(IIb)	0.1719(42)	0.1719(2)	0.1719(2)	0.0340	12.15
w1	0.4480(6)	0.0755(3)	0.0755(8)	0.0830	9.50
w2	0.6250	0.1250	0.3088(4)	0.0830	7.34
w3	0.4066(1)	0.2647(4)	0.2647(2)	0.0570	7.34
w4	0.3089(1)	-0.0588(1)	-0.0588(1)	0.0600	4.82

AgY760-250					
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0360(1)	0.3044(1)	0.1239(1)	0.9000	2.03
O1	0.0000	0.3557(1)	0.1442(1)	1.0000	2.78
O2	-0.0034(1)	0.2533(1)	0.1095(1)	1.0000	2.78
O3	0.0785(1)	0.2867(1)	0.1715(1)	1.0000	2.78
O4	0.0695(1)	0.3220(1)	0.0695(1)	1.0000	2.78
Ag(I)	0.0000	0.0000	0.0000	0.0500	12.15
Ag(I')	0.0657	0.0657	0.0657	0.0720	12.15
Ag(IIb)	0.1651	0.1651	0.1651	0.0300	12.15
w1	0.4575	0.0690	0.0690	0.0830	4.80
w2	0.6250	0.1250	0.3161	0.0832	4.80
w3	0.3913	0.2539	0.2539	0.0569	4.80
w4	0.2410	0.0091	0.0091	0.0433	4.80

AgY760-550					
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0366(1)	0.3044(1)	0.1234(1)	0.9000	2.14
O1	0.0000	0.3550(1)	0.1450(1)	1.0000	3.12
O2	-0.0027(1)	0.2527(1)	0.1099(1)	1.0000	3.12
O3	0.0805(1)	0.2872(1)	0.1695(1)	1.0000	3.12
O4	0.0680(1)	0.3228(1)	0.0681(1)	1.0000	3.12
Ag(I)	0.0000	0.0000	0.0000	0.0935	15.14
Ag(I')	0.0568	0.0568	0.0568	0.0670	15.14
Ag(IIb)	0.2188	0.2188	0.2188	0.0133	15.14
w1	0.4443	0.0900	0.0900	0.0509	11.87

AgY760-900					
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0364(1)	0.3045(1)	0.1233(1)	0.9000	3.86
O1	0.0000	0.3554(1)	0.1446(1)	1.0000	5.43
O2	-0.0027(1)	0.2527(1)	0.1101(2)	1.0000	5.43
O3	0.0807(1)	0.2878(2)	0.1692(1)	1.0000	5.43
O4	0.0675(1)	0.3229(1)	0.0675(1)	1.0000	5.43
Ag(I)	0.0000	0.0000	0.0000	0.0920	12.5
Ag(I')	0.0588(1)	0.0588(1)	0.0588(1)	0.0710	12.5
Ag(IIb)	0.2308(8)	0.2308(8)	0.2308(6)	0.0100	12.5

Tables SI3. Framework atomic coordinates, site occupancy, and atomic displacement parameters, ADPs (U_{iso}* = U_i/U_e*100 [Å^{-2}]) for the investigated AgY760 PFOA loaded zeolite at 25, 200, 250, 550, 700°C *in situ* heating.

	AgY760-PFOA-25				
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0359(1)	0.30374(9)	0.1247(1)	0.9000	0.66
O1	0.0000	0.3559(1)	0.1440(1)	1.0000	1.65
O2	-0.0036(1)	0.2535(1)	0.1089(2)	1.0000	1.65
O3	0.0763(1)	0.2853(1)	0.1736(1)	1.0000	1.65
O4	0.0715(1)	0.3205(1)	0.0715(1)	1.0000	1.65
C1	0.2610	0.3400	0.3005	0.0751	14.52
C2	0.2193	0.3772	0.3005	0.0751	14.52
C3	0.2240	0.4187	0.2635	0.0751	14.52
C5	0.1409	0.4160	0.3341	0.1502	14.52
C4	0.3400	0.1810	0.3800	0.0751	14.52
F1	0.4258	0.1190	0.3800	0.2816	14.52
F2	0.1400	0.4494	0.3005	0.5632	14.52
H1	0.2800	0.4494	0.2487	0.0563	14.52
O1n	0.3005	0.4494	0.2200	0.0931	14.52
Ag(I)	0.0000	0.0000	0.0000	0.0215	10.25
Ag(I')	0.1852	0.1852	0.1852	0.0638	10.25
Ag(IIb)	0.2368	0.2368	0.2368	0.0330	10.25
w1	0.6267	0.0524	0.0524	0.2049	5.04
w2	0.6250	0.1250	0.2688	0.1531	5.04
w3	0.4753	0.1854	0.1854	0.1658	5.04
w4	0.2970	-0.0469	-0.0469	0.2051	5.04

AgY760-PFOA-200					
Site	***x*/a**	***y*/b**	***z*/c**	**Fraction**	**Ui/Ue*100**
T	0.0361(1)	0.3036(1)	0.1250(1)	0.9000	0.66
O1	0.0000	0.3557(1)	0.1442(1)	1.0000	1.65
O2	-0.0035(1)	0.2535(1)	0.1095(2)	1.0000	1.65
O3	0.0766(1)	0.2855(2)	0.1733(1)	1.0000	1.65
O4	0.0713(1)	0.3203(2)	0.0713(1)	1.0000	1.65
C1	0.2610	0.3400	0.3005	0.0681	14.68
C2	0.2193	0.3772	0.3005	0.0681	14.68
C3	0.2240	0.4187	0.2635	0.0681	14.68
C5	0.1409	0.4160	0.3341	0.1362	14.68
C4	0.3400	0.1810	0.3800	0.0681	14.68
F1	0.4258	0.1190	0.3800	0.2554	14.68
F2	0.1400	0.4494	0.3005	0.5107	14.68
H1	0.2800	0.4494	0.2487	0.0511	14.68
O1n	0.3005	0.4494	0.2200	0.1013	14.68
Ag(I)	0.0000	0.0000	0.0000	0.0266	11.90
Ag(I')	0.0577	0.0577	0.0577	0.0610	11.90
Ag(IIb)	0.1904	0.1904	0.1904	0.0350	11.90
w1	0.6336	0.0853	0.0853	0.0249	8.40

AgY760-PFOA-250					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0361(1)	0.3039(1)	0.1244(1)	0.9000	0.87
O1	0.0000	0.3556(1)	0.1443(1)	1.0000	1.96
O2	-0.0033(1)	0.2532(1)	0.1097(2)	1.0000	1.96
O3	0.0779(1)	0.2863(1)	0.1720(1)	1.0000	1.96
O4	0.0700(1)	0.3210(1)	0.0700(1)	1.0000	1.96
C1	0.2610	0.3400	0.3005	0.0559	15.00
C2	0.2193	0.3772	0.3005	0.0559	15.00
C3	0.2240	0.4187	0.2635	0.0559	15.00
C5	0.1409	0.4160	0.3341	0.1118	15.00
C4	0.3400	0.1810	0.3800	0.0559	15.00
F1	0.4258	0.1190	0.3800	0.2096	15.00
F2	0.1400	0.4494	0.3005	0.4193	15.00
H1	0.2800	0.4494	0.2487	0.0419	15.00
O1n	0.3005	0.4494	0.2200	0.0838	15.00
Ag(I)	0.0000	0.0000	0.0000	0.0340	12.05
Ag(I')	0.0583	0.0583	0.5830	0.0590	12.05
Ag(IIb)	0.1887	0.1887	0.1887	0.0330	12.05
w1	0.6014	0.0747	0.0747	0.0205	8.82

AgY760-PFOA-550					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0363(1)	0.3045(1)	0.1235(1)	0.9000	0.95
O1	0.0000	0.3557(1)	0.1442(1)	1.0000	2.32
O2	-0.0029(1)	0.2529(1)	0.1099(1)	1.0000	2.32
O3	0.0796(1)	0.2875(1)	0.1703(1)	1.0000	2.32
O4	0.0684(1)	0.3227(1)	0.0684(1)	1.0000	2.32
Ag(I)	0.0000	0.0000	0.0000	0.0860	19.81
Ag(I')	0.0541(2)	0.0541(2)	0.0541(2)	0.1010	19.81

AgY760-PFOA-700					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0364(1)	0.3045(1)	0.1232(4)	0.9000	1.07
O1	0.0000	0.3554(1)	0.1445(1)	1.0000	2.62
O2	-0.0027(1)	0.2526(1)	0.1102(1)	1.0000	2.62
O3	0.0807(1)	0.2878(1)	0.1692(1)	1.0000	2.62
O4	0.0675(1)	0.3230(1)	0.0675(1)	1.0000	2.62
Ag(I)	0.0000	0.0000	0.0000	0.0860	20.10
Ag(I')	0.0509	0.0509	0.0509	0.1087	20.10

Tables SI4. Framework atomic coordinates, site occupancy, and atomic displacement parameters, ADPs (U_{iso}* = U_i/U_e*100 [$Å^{-2}$]) for the investigated AgY760 PFOS loaded zeolite heated at 25, 200, 250, 550, 800°C.

	AgY760-PFOS-25				
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0359(1)	0.3037(1)	0.1245(1)	0.9000	0.84
O1	0.0000	0.3558(1)	0.1441(1)	1.0000	1.60
O2	-0.0035(1)	0.2534(1)	0.1088(2)	1.0000	1.60
O3	0.0765(7)	0.2853(2)	0.1734(1)	1.0000	1.60
O4	0.0714(1)	0.3207(2)	0.0714(1)	1.0000	1.60
S	0.2219	0.4494	0.2000	0.0457	17.83
C1	0.2610	0.3400	0.3005	0.0610	17.83
C2	0.2193	0.3772	0.3005	0.0610	17.83
C3	0.2240	0.4187	0.2635	0.0610	17.83
C5	0.1409	0.4160	0.3341	0.1220	17.83
C4	0.3400	0.1810	0.3800	0.0610	17.83
F2	0.1400	0.4494	0.3005	0.4575	17.83
F1	0.4258	0.1190	0.3800	0.2288	17.83
H1	0.1400	0.4580	0.2400	0.0457	17.83
O1n	0.1600	0.4580	0.2600	0.0457	17.83
O2n	0.1800	0.4100	0.3005	0.0457	17.83
w1	0.5576	0.1071	0.1071	0.1458	8.12
w3	0.3688	0.2765	0.2765	0.2180	8.12
w4	0.3006	-0.0505	-0.0505	0.4766	8.12
Ag(I)	0.0000	0.0000	0.0000	0.0634	11.24
Ag(I')	0.0938	0.0938	0.0938	0.0507	11.24
Ag(IIb)	0.1907	0.1907	0.1907	0.0642	11.24

AgY760-PFOS-200					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0360(1)	0.3037(1)	0.1255(1)	0.9000	0.95
O1	0.0000	0.3562(1)	0.1437(1)	1.0000	1.74
O2	-0.0040(1)	0.2540(1)	0.1092(2)	1.0000	1.74
O3	0.0749(1)	0.2851(2)	0.1751(1)	1.0000	1.74
O4	0.0728(1)	0.3195(2)	0.0728(1)	1.0000	1.74
S	0.2219	0.4494	0.2000	0.0413	18.21
C1	0.2610	0.3400	0.3005	0.0550	18.21
C2	0.2193	0.3772	0.3005	0.0550	18.21
C3	0.2240	0.4187	0.2635	0.0550	18.21
C5	0.1409	0.4160	0.3341	0.1100	18.21
C4	0.3400	0.1810	0.3800	0.0550	18.21
F2	0.1400	0.4494	0.3005	0.4125	18.21
F1	0.4258	0.1190	0.3800	0.2063	18.21
H1	0.1400	0.4580	0.2400	0.0413	18.21
O1n	0.1600	0.4580	0.2600	0.0413	18.21
O2n	0.1800	0.4100	0.3005	0.0413	18.21
w1	0.5716	0.1440	0.1440	0.0674	9.57
w3	0.3186	0.2931	0.2931	0.1004	1.10
Ag(I)	0.0000	0.0000	0.0000	0.0690	13.44
Ag(I')	0.0710	0.0710	0.0710	0.0680	13.44
Ag(IIb)	0.1854	0.1854	0.1854	0.0400	13.44

AgY760-PFOS-250					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0360(1)	0.3038(1)	0.1253(1)	0.9000	0.99
O1	0.0000	0.3561(1)	0.1438(1)	1.0000	1.78
O2	-0.0038(1)	0.2538(1)	0.1094(2)	1.0000	1.78
O3	0.0756(1)	0.2854(2)	0.1743(1)	1.0000	1.78
O4	0.0721(1)	0.3200(2)	0.0721(1)	1.0000	1.78
S	0.2219	0.4494	0.2000	0.0376	18.24
C1	0.2610	0.3400	0.3005	0.0501	18.24
C2	0.2193	0.3772	0.3005	0.0501	18.24
C3	0.2240	0.4187	0.2635	0.0501	18.24
C5	0.1409	0.4160	0.3341	0.1002	18.24
C4	0.3400	0.1810	0.3800	0.0501	18.24
F2	0.1400	0.4494	0.3005	0.3758	18.24
F1	0.4258	0.1190	0.3800	0.1879	18.24
H1	0.1400	0.4580	0.2400	0.0376	18.24
O1n	0.1600	0.4580	0.2600	0.0376	18.24
O2n	0.1800	0.4100	0.3005	0.0376	18.24
w1	0.5729	0.1475	0.1475	0.0639	9.80
w3	0.3178	0.2908	0.2908	0.0815	7.97
Ag(I)	0.0000	0.0000	0.0000	0.0735	14.21
Ag(I')	0.0684	0.0684	0.0684	0.0831	14.21
Ag(IIb)	0.1862	0.1862	0.1862	0.0273	14.21

AgY760-PFOS-550					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0361(1)	0.3044(1)	0.1239(1)	0.9000	1.51
O1	0.0000	0.3561(1)	0.1438(1)	1.0000	2.46
O2	-0.0034(1)	0.2533(1)	0.1098(2)	1.0000	2.46
O3	0.0784(1)	0.2872(2)	0.1715(1)	1.0000	2.46
O4	0.0694(1)	0.3219(2)	0.0694(1)	1.0000	2.46
S	0.2219	0.4494	0.2000	0.0080	22.01
C1	0.2610	0.3400	0.3005	0.0107	22.01
C2	0.2193	0.3772	0.3005	0.0107	22.01
C3	0.2240	0.4187	0.2635	0.0107	22.01
C5	0.1409	0.4160	0.3341	0.0214	22.01
C4	0.3400	0.1810	0.3800	0.0107	22.01
F2	0.1400	0.4494	0.3005	0.0803	22.01
F1	0.4258	0.1190	0.3800	0.0401	22.01
H1	0.1400	0.4580	0.2400	0.0080	22.01
O1n	0.1600	0.4580	0.2600	0.0080	22.01
O2n	0.1800	0.4100	0.3005	0.0080	22.01
Ag(I)	0.0000	0.0000	0.0000	0.0863	18.00
Ag(I')	0.0616	0.0616	0.0616	0.0777	18.00
Ag(IIb)	0.1843	0.1843	0.1843	0.0183	18.00

AgY760-PFOS-800					
Site	**x/a**	**y/b**	**z/c**	**Fraction**	**Ui/Ue*100**
T	0.0363(2)	0.3045(2)	0.1234(1)	0.9000	1.16
O1	0.0000	0.3557(1)	0.1442(1)	1.0000	2.08
O2	-0.0028(5)	0.2528(1)	0.1101(1)	1.0000	2.08
O3	0.0800(1)	0.2878(1)	0.1700(1)	1.0000	2.08
O4	0.0680(1)	0.3226(1)	0.0680(1)	1.0000	2.08
Ag(I)	0.0000	0.0000	0.0000	0.0991	20.96
Ag(I')	0.0595	0.0595	0.0595	0.0785	20.96
Ag(IIb)	0.2380	0.2380	0.2380	0.0137	20.96

Table SI5. Framework atomic bond distances and angles for AgY760 at 25, 200, 250, 550, and 900 °C.

	AgY760-25	**AgY760-200**	**AgY760-250**	**AgY760-550**	**AgY760-900**
Bond(Å)			Value (Å)		
T-O1	1.605(2)	1.601(2)	1.600(2)	1.601(2)	1.599(2)
T-O2	1.602(2)	1.604(2)	1.603(2)	1.608(2)	1.604(2)
T-O3	1.603(2)	1.606(2)	1.605(2)	1.600(2)	1.599(2)
T-O4	1.605(2)	1.607(2)	1.608(2)	1.607(2)	1.610(2)
MeanValue	1.604	1.605	1.604	1.604	1.603
Angle(°)			Value (°)		
O1-*T*-O2	109.8(2)	109.9(2)	110.0(2)	109.6(2)	109.9(2)
O1-*T*-O3	109.5(2)	109.6(2)	109.6(2)	109.8(2)	109.9(2)
O1-*T*-O4	108.6(2)	108.8(2)	108.7(2)	108.9(2)	108.4(2)
O2-*T*-O3	109.6(2)	109.4(2)	109.4(2)	109.5(2)	109.6(2)
O2-*T*-O4	109.3(2)	109.2(2)	109.2(2)	109.1(2)	108.9(2)
O3-*T*-O4	109.9(2)	109.6(2)	109.6(2)	109.8(2)	109.8(2)
MeanValue	109.5	109.4	109.4	109.5	109.4
T-O1-*T*	141.2(4)	141.4(4)	141.1(4)	143.9(4)	143.1(4)
T-O2-*T*	150.0(3)	150.4(4)	150.9(3)	151.9(4)	152.1(4)
T-O3-*T*	147.4(3)	147.6(3)	148.4(3)	149.6(4)	150.5(4)
T-O4-T	139.5(2)	139.6(2)	139.3(2)	135.7(2)	135.1(2)
MeanValue	144.5	144.8	144.9	145.3	145.2

Table SI6. Framework atomic bond distances and angles for AgY760-PFOA at 25, 200, 250, 550, and 700 °C.

Bond(Å)	**AgY760-PFOA-25**	**AgY760-PFOA-200**	**AgY760-PFOA-250**	**AgY760-PFOA-550**	**AgY760-PFOA-700**
T-O1	1.607(2)	1.609(2)	1.606(2)	1.603(2)	1.602(2)
T-O2	1.596(2)	1.597(2)	1.599(2)	1.603(2)	1.603(2)
T-O3	1.602(2)	1.592(2)	1.595(2)	1.601(2)	1.598(2)
T-O4	1.608(2)	1.609(2)	1.610(2)	1.607(2)	1.609(2)
MeanValue	1.603	1.602	1.603	1.604	1.603
Angle(°)			Value(°)		
O1-*T*-O2	110.2(2)	109.7(2)	109.9(2)	110.0(1)	109.8(1)
O1-*T*-O3	109.6(2)	109.8(2)	109.8(2)	109.6(1)	109.8(1)
O1-*T*-O4	108.9(2)	109.0(2)	108.8(2)	108.2(1)	108.2(2)
O2-*T*-O3	109.5(2)	109.6(2)	109.6(2)	109.5(2)	109.6(2)
O2-*T*-O4	108.7(2)	108.7(2)	108.7(2)	109.3(2)	109.2(2)
O3-*T*-O4	109.6(2)	109.7(2)	109.8(2)	109.9(2)	109.9(2)
MeanValue	109.4	109.4	109.4	109.4	109.4
T-O1-*T*	138.9(4)	139.1(4)	140.2(4)	141.9(3)	143.1(3)
T-O2-*T*	149.0(4)	149.7(4)	150.6(4)	151.8(3)	152.4(3)
T-O3-*T*	146.0(3)	146.5(4)	148.0(4)	150.0(3)	150.7(3)
T-O4-T	143.0(2)	142.6(3)	140.4(3)	136.8(2)	134.9(2)
MeanValue	144.2	144.5	144.8	145.1	145.3

Table SI7. Framework atomic bond distances and angles for AgY760-PFOS at 25, 200, 250, 550, and 800 °C.

Bond(Å)	**AgY760-PFOS-25**	**AgY760-PFOS-200**	**AgY760-PFOS-250**	**AgY760-PFOS-550**	**AgY760-PFOS-800**
T-O1	1.609(2)	1.607(2)	1.606(2)	1.605(2)	1.604(2)
T-O2	1.596(2)	1.600(2)	1.601(2)	1.603(2)	1.604(2)
T-O3	1.606(2)	1.594(2)	1.593(2)	1.599(2)	1.600(2)
T-O4	1.604(2)	1.607(2)	1.608(2)	1.607(2)	1.607(2)
MeanValue	1.604	1.602	1.602	1.604	1.604
Angle(°)			Value(°)		
O1-*T*-O2	110.2(2)	109.6(2)	109.7(2)	109.8(2)	110.0(1)
O1-*T*-O3	109.4(2)	109.8(2)	110.0(2)	109.7(2)	109.6(1)
O1-*T*-O4	109.0(2)	109.3(2)	109.1(2)	108.3(2)	108.2(2)
O2-*T*-O3	109.3(2)	109.4(2)	109.4(2)	109.6(2)	109.6(2)
O2-*T*-O4	109.1(2)	108.6(2)	108.6(2)	109.1(2)	109.2(2)
O3-*T*-O4	109.6(2)	109.7(2)	109.8(2)	110.0(2)	110.0(2)
MeanValue	109.4	109.4	109.4	109.4	109.4
T-O1-*T*	139.4(4)	136.9(4)	137.6(4)	140.3(4)	142.0(3)
T-O2-*T*	149.2(4)	148.8(4)	149.3(4)	151.5(4)	152.1(3)
T-O3-*T*	146.1(4)	144.4(4)	145.3(4)	149.0(4)	150.5(3)
T-O4-T	142.76(31)	145.9(3)	144.4(3)	139.0(3)	136.3(2)
MeanValue	144.4	144.0	144.2	145.0	145.2

Table SI8. Extraframework atomic bond distances for AgY760 at 25, 200, 250, 550, and 900 °C.

AgY760-25	
Distance	Value(Å)
w1-w1	2.49(1)
w1-w3	2.39(5)
w1-w3[x2]	3.32(3)
w2-w3[x3]	3.38(4)
w3-O4	2.94(1)
w3-w4	2.99(1)
w4-w3	2.99(1)
Ag(I)-O3[x6]	3.11(4)
Ag(I)-Ag(IIb)[x3]	3.10(1)
Ag(I')-O2[x3]	3.11(4)
Ag(I')-O3[x3]	2.67(4)
Ag(I')-Ag(IIb)[x3]	2.82(1)
Ag(IIb)-O2[x3]	2.49(4)
Ag(IIb)-O4[x3]	3.24(4)

AgY760-200	
Distance	Value(Å)
w1-O4	3.06(4)
w1-O1[x2]	3.35(10)
w1-w2	1.71(13)
w1-w3[x2]	2.23(12)
w1-w3[x2]	3.26(16)
w2-w3[x4]	3.31(11)
w3-w3[x2]	2.70(2)
w3-w4	2.82(2)
Ag(I)-O3[x6]	2.83(1)
Ag(I)-Ag(I')	2.84(5)
Ag(I')-O2[x3]	3.02(1)
Ag(I')-O3[x3]	2.56(5)
Ag(I')-Ag(IIb)[x3]	2.56(8)
Ag(IIb)-O2[x3]	2.90(1)

AgY760-250	
Distance	Value(Å)
w1-w2	2.01(2)
w1-w3[x2]	2.17(2)
w1-w3	2.97(3)
w2-w1	2.00(2)
w2-O4[x2]	3.31(1)
w3-O4	3.02(1)
w4-O2[x3]	2.48(1)
w4-O4	2.86(1)
w4-O4[x2]	2.86(1)
Ag(I)-O3[x6]	2.84(1)
Ag(I)-Ag(I')	2.76(3)
Ag(I')-O2[x3]	2.53(1)
Ag(I')-O3[x3]	2.98(2)
Ag(I')-Ag(IIb)[x3]	2.50(1)
Ag(IIb)-O2[x3]	3.09(1)
Ag(IIb)-Ag(IIb)[x3]	2.75(1)
Ag(IIb)-w4	3.19(1)

AgY760-550	
Distance	Value(Å)
w1-O4	3.04(1)
w1-w1	2.40(1)
Ag(I)-O2[x6]	3.40(1)
Ag(I)-O3[x6]	2.90(5)
Ag(I)-Ag(I')	2.38(3)
Ag(I')-O2[x3]	2.87(3)
Ag(I')-O3[x3]	2.42(1)
Ag(IIb)-O2[x3]	2.23(5)
Ag(IIb)-O4[x3]	2.82(2)

AgY760-900	
Distance	Value(Å)
Ag(I')-O2[x3]	2.88(1)
Ag(I')-O4[x3]	2.46(1)
Ag(I)-O3[x6]	2.91(3)
Ag(I)-Ag(I')[x2]	2.47(5)
Ag(IIb)-O2[x3]	2.33(8)
Ag(IIb)-O4[x3]	2.78(3)

Table SI9. Extraframework atomic bond distances for AgY760-PFOA at 25, 200, 250, 550, and 700 °C.

AgY760-PFOA-25	
Distance	Value(Å)
O1-F1	1.86(1)
O3-F1	2.29(4)
O4-C5	1.76(1)
O4-F1	1.84(4)
w1-w1[x2]	2.43(1)
w1-w1[x2]	2.55(3)
w1-w2	2.47(2)
w1-w3[x2]	2.42(1)
w1-w4[x3]	1.86(3)
w1-C1[x2]	2.23(3)
w1-C2[x2]	2.02(3)
w1-C3[x2]	2.39(2)
w2-w3	2.08(1)
w2-O1n	2.57(1)
w2-O1n	2.57(4)
w3-C2	1.46(2)
w3-C4	1.83(2)
w3-F2	2.12(4)
w3-H1	2.11(1)
w4-Ag(IIb)	2.53(1)
Ag(I)-O3[x6]	2.76(1)
Ag(I')-O4[x3]	3.29(2)
Ag(I')-Ag(IIb)[x3]	2.17(2)
Ag(IIb)-O2[x3]	2.58(1)
Ag(IIb)-O2[x3]	2.39(3)
Ag(IIb)-O4[x3]	2.85(3)

AgY760-PFOA-200	
Distance	Value(Å)
O1-F1	1.86(1)
O3-F1	2.28(3)
O4-C5	1.77(1)
O4-F2	1.83(4)
w1-C1[x2]	2.41(3)
w1-C1[x2]	2.09(3)
w1-w1[x4]	2.38(1)
w1-w1[x2]	1.66(1)
w1-w1[x2]	1.97(1)
Ag(I)-O3[x6]	2.77(1)
Ag(I)-Ag(I')[x2]	2.43(4)
Ag(I')-O3[x3]	2.91(3)
Ag(I')-O2[x3]	2.36(3)
Ag(I')-Ag(IIb)[x3]	3.22(1)
Ag(IIb)-O2[x3]	2.48(1)
Ag(IIb)-O4[x3]	3.18(1)

AgY760-PFOA-250	
Distance	Value(Å)
O1-F1	1.86(1)
O3-F1	2.25(3)
O4-C5	1.76(2)
O4-F2	1.80(2)
w1-C1[x2]	2.18(2)
w1-w1[x2]	2.53(3)
Ag(I)-O3[x6]	2.82(1)
Ag(I)-Ag(I')[x2]	2.45(3)
Ag(I')-O2[x3]	2.90(5)
Ag(I')-O3[x3]	2.39(1)
Ag(I')-Ag(IIb)[x3]	3.17(1)
Ag(IIb)-O2[x3]	2.51(1)

AgY760-PFOA-550	
Distance	Value(Å)
Ag(I)-O3[x6]	2.88(1)
Ag(I)-Ag(I')[x3]	2.27(9)
Ag(I')-O2[x3]	2.85(1)
Ag(I')-O3[x3]	2.38(2)

AgY760-PFOA-700	
Distance	Value(Å)
Ag(I)-O3[x6]	2.91(4)
Ag(I)-Ag(I')[x3]	2.13(2)
Ag(I')-O2[x3]	2.83(1)
Ag(I')-O3[x3]	2.38(1)

Table SI10. Extraframework atomic bond distances for AgY760-PFOS at 25, 200, 250, 550, and 800 °C.

AgY760-PFOS-25	
Distance	Value(Å)
O1-F1	1.86(1)
O1-O2n	2.54(4)
O3-F1	2.30(1)
O4-C5	1.75(1)
O4-F2	1.83(1)
O4-F1	1.84(2)
w1-w1	1.70(1)
w1-w1[x4]	2.55(1)
w1-w3[x2]	2.17(2)
w1-C1[x2]	2.19(2)
w3-C1[x2]	2.29(2)
w3-C2[x2]	1.52(1)
w3-C3[x2]	1.79(1)
w3-H1	1.79(1)
w3-O1n	2.13(2)
w3-w4[x3]	1.85(2)
w4-C1[x6]	1.36(1)
Ag(I)-O3[x6]	2.76(5)
Ag(I')-O3[x3]	3.19(1)
Ag(I')-Ag(I')[x3]	2.14(2)
Ag(IIb)-O2[x3]	2.47(1)
Ag(IIb)-O4[x3]	3.19(1)
Ag(IIb)-Ag(I')[x3]	2.63(3)

AgY760-PFOS-200	
Distance	Value(Å)
O1-F1	1.86(1)
O1-O2n	2.53(1)
O3-F1	2.31(5)
O4-C5	1.77(5)
O4-F1	1.83(5)
O4-F2	1.87(4)
w1-w1[x4]	2.15(3)
w1-w1[x2]	2.48(2)
w1-w3[x2]	2.48(2)
w1-C1[2]	2.39(1)
w3-C1	1.81(1)
w3-C2	2.29(1)
Ag(I)-O3[x6]	2.71(1)
Ag(I)-Ag(I')[x3]	2.98(4)
Ag(I')-O3[x3]	3.08(2)
Ag(I')-O2[x3]	2.58(1)
Ag(I')-Ag(IIb)[x3]	2.78(4)
Ag(IIb)-O2[x3]	3.27(1)
Ag(IIb)-O4[x3]	2.59(2)

AgY760-PFOS-250	
Distance	Value(Å)
O1-F1	1.86(1)
O1-O2n	2.53(4)
O3-F1	2.29(5)
O4-C5	1.77(1)
O4-F1	1.84(2)
O4-F2	1.85(3)
w1-w1[x4]	2.23(1)
w1-w1[x2]	2.56(1)
w1-w3[x2]	2.57(1)
w1-C1[x2]	2.41(1)
w3-C1[x2]	1.84(1)
w3-C2[x2]	2.27(1)
Ag(I)-O3[x6]	2.74(1)
Ag(I)-Ag(I')[x3]	2.87(3)
Ag(I')-O3[x3]	2.53(3)
Ag(IIb)-O2[x3]	2.57(3)
Ag(IIb)-Ag(I')[x3]	2.86(4)

AgY760-PFOS-550	
Distance	Value(Å)
O1-F1	1.86(1)
O1-O2n	2.53(4)
O3-F1	2.23(1)
O4-C5	1.75(1)
O4-F1	1.86(4)
O4-F2	1.77(2)
Ag(I)-O3[x6]	2.84(1)
Ag(I)-Ag(I')[x3]	2.58(1)
Ag(I')-O2[x3]	2.93(3)
Ag(I')-O3[x3]	2.46(5)
Ag(I')-Ag(IIb)[x3]	2.98(1)
Ag(IIb)-O2[x3]	2.60(1)

AgY760-PFOS-800	
Distance	Value(Å)
Ag(I)-O3[x6]	2.89(2)
Ag(I)-Ag(I')[x3]	2.50(1)
Ag(I')-O2[x3]	2.90(1)
Ag(I')-O3[x3]	2.46(2)
Ag(IIb)-O2[x3]	2.43(3)
Ag(IIb)-O4[x3]	2.81(1)

Table SI11. Thermally induced evolution of O1-O1 and O4-O4 diameters for the 12MR apertures of zeolite Y channels in AgY760, AgY760-PFOA and AgY760-PFOS.

Sample	O1-O1 (Å)	O4-O4 (Å)	Diameter (Å)	C.F.A. (Å²)	ε*
AgY760-25	9.91	9.88	7.20	40.68	1.00
AgY760-200	9.92	9.89	7.20	40.72	1.00
AgY760-250	9.90	9.87	7.19	40.53	1.00
AgY760-550	9.95	9.78	7.17	40.31	0.98
AgY760-900	9.91	9.74	7.13	39.86	0.98
AgY760-PFOA-25	9.89	10.00	7.24	41.19	1.01
AgY760-PFOA-200	9.91	10.00	7.26	41.34	1.01
AgY760-PFOA-250	9.91	9.93	7.22	40.89	1.00
AgY760-PFOA-550	9.89	9.79	7.14	40.03	0.99
AgY760-PFOA-700	9.91	9.74	7.12	39.85	0.98
AgY760-PFOS-25	9.90	9.99	7.24	41.19	1.01
AgY760-PFOS-200	9.87	10.09	7.28	41.58	1.02
AgY760-PFOS-250	9.87	10.04	7.26	41.36	1.02
AgY760-PFOS-550	9.87	9.86	7.17	40.34	1.00
AgY760-PFOS-800	9.89	9.78	7.14	39.98	0.99