

TABLE S3. Rietveld refinement statistics, calculated unit cell and structural parameters of the GD4a erionite sample.

Crystal system = Hexagonal; space group = $P6_3/mmc$							
Temperature (K) = 293							
$a = 13.2323(6)\text{\AA}$; $c = 15.0662(8)\text{\AA}$							
$V = 2284.57(2)\text{\AA}^3$							
$Z = 1$							
Radiation type lab ($\lambda = 1.5418\text{\AA}$) and synchrotron ($\lambda = 0.8263\text{\AA}$)							
Merged $R_{wp} = 6.89\%$; $R_p = 5.21\%$; $\chi^2 = 3.875$							
Merged number of observations = 2389							
No. of parameters = 111							
No. of restraints = 8							
Merged $R[F^2] = 14.91\%$							
Site	Site multiplicity	x	y	z	U_{iso}	Site occupancy	Proposed atom assignment
Framework							
T1	24	-0.00297(13)	0.23122(14)	0.10459(18)	0.0358(4)	1	Si = 0.79, Al = 0.21
T2	12	0.08922(15)	0.42292(19)	0.25	0.0212(5)	1	Si = 0.79, Al = 0.21
O1	24	-0.03415(18)	0.31894(15)	0.65617(20)	0.0118(5)	1	O = 1
O2	12	0.10250(23)	0.20450(29)	0.11032(17)	0.0592(5)	1	O = 1
O3	12	0.12286(18)	0.24572(15)	0.65479(12)	0.0577(4)	1	O = 1
O4	12	0.26359(13)	0	0	0.0430(5)	1	O = 1
O5	6	0.23184(21)	0.46368(18)	0.25	0.0549(7)	1	O = 1
O6	6	0.08440(13)	0.54220(20)	0.25	0.0198(5)	1	O = 1
Extraframework							
Ca1	4	0.333333	0.666667	0.8733(6)	0.012(5)	0.141(6)	Ca = 0.1414
Na1	4	0.333333	0.666667	0.8733(6)	0.012(5)	0.0937*	Na = 0.0937*
Ca2	4	0.666667	0.333333	0.2243(8)	0.012(7)	0.195(7)	Ca = 0.1954
Ba2	4	0.666667	0.333333	0.2243(8)	0.012(7)	0.0063*	Ba = 0.0063*
K1	2	0	0	0.25	0.038(5)	0.931(8)	K = 0.9314
K2	6	0.5	0	0	0.068(6)	0.026(7)	K = 0.0264
K3	4	0.333333	0.666667	0.1135(5)	0.010(6)	0.136(6)	K = 0.1365

Mg1	4	0.666667	0.333333	-0.0344(7)	0.075(8)	0.246(9)	Mg = 0.2464
Water molecules							
OW1	12	0.2649(5)	0.5299(6)	0.0415(7)	0.013(4)	0.207(6)	O = 0.2075
OW2	12	0.2390(5)	0.4781(6)	0.7023(5)	0.012(7)	0.427(6)	O = 0.4272
OW3	24	0.2362(6)	0.5618(6)	0.5722(8)	0.010(4)	0.306(8)	O = 0.3059
OW4	12	0.4708(5)	0.9416(9)	0.9329(6)	0.072(4)	0.327(6)	O = 0.3272
OW5	12	0.4390(6)	-0.122(1)	0.034(1)	0.014(6)	0.411(8)	O = 0.2057
OW6	12	0.4406(5)	0.8813(4)	0.8416(5)	0.051(4)	0.406(6)	O = 0.4062
OW7	12	0.403(1)	0.806(1)	0.101(1)	0.045(8)	0.065(9)	O = 0.4062

*fixed to the a.f.u. from the formula calculated from the EPMA data.