Supplementary information

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1 – Bond Lengths and Angles

Table 1 *– Bond Distances (Å) and Angles (deg) in ITQ-29 from 100–300 K (errors at 1σ level).*

Bond Length/Angle	Temperature										
	300K	**280K**	**260K**	**240K**	**220K**	**200K**	**180K**	**160K**	**140K**	**120K**	**100K**
Si – O1	1.609(4)	1.615(4)	1.615(4)	1.615(4)	1.614(4)	1.613(4)	1.613(5)	1.609(4)	1.605(5)	1.59(1)	1.59(1)
Si – O2	1.578(4)	1.578(4)	1.578(4)	1.579(4)	1.579(4)	1.580(4)	1.580(5)	1.579(4)	1.577(5)	1.59(1)	1.58(1)
Si – O3	1.589(3)	1.585(3)	1.586(3)	1.587(3)	1.587(3)	1.586(3)	1.588(3)	1.592(3)	1.599(3)	1.613(7)	1.616(9)
Si – O1 – Si	146.2(6)	144.1(6)	144.6(6)	145.2(6)	145.7(6)	146.5(6)	146.2(8)	150.1(7)	152.0(8)	152.6(2)	155.7(2)
Si – O2 – Si	162.6(5)	164.3(5)	163.7(5)	163.0(5)	162.3(5)	161.4(5)	161.8(7)	158.2(5)	157.2(7)	155.6(2)	158.4(2)
Si – O3 – Si	152.3(4)	153.0(5)	153.8(5)	152.6(4)	152.5(4)	152.4(5)	152.4(6)	151.8(5)	151.2(6)	148.7(1)	146.9(2)
O1 – Si – O2	109.4(4)	109.2(4)	109.1(4)	109.1(4)	109.0(4)	109.0(4)	109.0(5)	109.2(4)	109.6(6)	109.1(1)	112.1(2)
O1 – Si – O3	108.7(3)	109.0(3)	108.3(3)	108.9(3)	108.8(3)	108.7(3)	108.7(3)	108.1(3)	107.6(4)	105.12(7)	105.7(9)
O2 – Si – O3	110.9(3)	110.8(3)	110.9(3)	111.0(3)	111.1(3)	111.2(3)	111.2(3)	111.8(3)	111.7(3)	111.05(7)	109.4(9)
O3 – Si – O3	108.2(4)	107.9(3)	107.9(5)	108.0(5)	108.0(5)	108.0(5)	108.0(6)	107.8(5)	108.(6)	114.9(1)	114.6(2)
Lattice Parameter (Å)	11.8532(1)	11.8535(1)	11.8550(1)	11.8572(1)	11.8580(1)	11.8603(1)	11.8602(2)	11.8635(1)	11.8661(2)	11.870(3)	11.872(4)
Unit Cell Volume (Å)	1665.34(5)	1665.49(5)	1666.12(5)	1667.05(5)	1667.38(5)	1668.34(5)	1668.30(6)	1669.68(6)	1670.79(7)	1672.3(1)	1673.4(2)

Table 2 *– Bond Distances (Å) and Angles (deg) in Dehydrated Ag-A from 100–300 K (errors at 1σ level).*

Bond Length/Angle	Temperature										
	300K	280K	260K	240K	220K	200K	180K	160K	140K	120K	100K
Si – O1	1.63(3)	1.63(2)	1.63(2)	1.62(2)	1.62(2)	1.62(2)	1.62(2)	1.62(2)	1.62 (2)	1.64(2)	1.61 (2)
Si – O2	1.55(3)	1.53(1)	1.54(1)	1.53(1)	1.53(1)	1.52(1)	1.52(1)	1.52(1)	1.52(1)	1.52(1)	1.51 (1)
Si – O3	1.62(1)	1.614(8)	1.620(9)	1.626(8)	1.619(8)	1.628(8)	1.628(8)	1.629(8)	1.630(8)	1.633(8)	1.639(8)
Al – O1	1.72(3)	1.72(2)	1.71 (2)	1.71 (2)	1.70(2)	1.70(2)	1.70(2)	1.70(2)	1.69(2)	1.68(2)	1.70(2)
Al – O2	1.75(3)	1.77(1)	1.76(1)	1.76(1)	1.75(1)	1.77(1)	1.77(1)	1.77(1)	1.77(1)	1.77(1)	1.78(1)
Al – O3	1.73(1)	1.736(8)	1.730(9)	1.735(8)	1.747(8)	1.737(8)	1.737(9)	1.738(8)	1.739(8)	1.733(8)	1.726(8)
Si – O1 – Al	148.8(9)	149.1(5)	149.7(5)	151.0(5)	152.3(5)	152.5(5)	152.4(5)	152.6(5)	152.9(5)	153.4(5)	154.4(5)
Si – O2 – Al	153.4(2)	153.3(9)	153.3(9)	153.3(9)	153.2(9)	153.5(8)	153.5(9)	153.6(8)	153.9(8)	153.9(9)	153.6(8)
Si – O3 – Al	149.6(9)	149.5(5)	149.6(5)	149.3(5)	149.1(5)	149.2(5)	149.1(5)	149.1(5)	148.7(5)	148.6(5)	149.1(5)
O1 – Si – O2	106(1)	106.1(7)	106.3(7)	106.7(7)	107.1(7)	107.8(6)	107.5(6)	107.8(6)	108.1(6)	108.6(6)	109.0(6)
O1 – Si – O3	109.5(6)	109.7(3)	109.3(3)	109.3(3)	109.0(3)	108.9(3)	108.9(3)	108.9(3)	108.7(3)	108.4(3)	107.8(3)
O2 – Si – O3	112.5(7)	112.5(4)	112.6(4)	112.5(4)	112.3(4)	112.4(4)	112.4(4)	112.4(4)	112.2(4)	112.3(4)	113.0(4)
O3 – Si – O3	106(1)	106.6(6)	106.6(6)	106.6(6)	107.1(6)	106.5(6)	106.6(6)	106.5(6)	106.7(6)	106.7(6)	106.0(6)
O1 – Al – O2	106(1)	106.4(6)	106.7(6)	107.6(6)	108.4(6)	108.4(6)	108.4(6)	108.4(6)	108.7(6)	108.7(6)	109.0(6)
O1 – Al – O3	110.2(6)	110.1(3)	110.1(3)	110.0(3)	109.5(3)	109.7(3)	109.7(3)	109.7(3)	109.8(3)	109.9(3)	109.8(3)
O2 – Al – O3	111.3(7)	111.3(4)	111.3(4)	111.1(4)	111.2(4)	111.0(4)	110.9(4)	110.9(4)	110.5(4)	110.3(4)	110.3(4)
O3 – Al – O3	108(1)	107.5(6)	107.5(6)	107.2(6)	107.1(6)	107.2(6)	107.3(6)	107.3(6)	107.5(6)	107.7(6)	107.7(6)
Lattice Parameter (Å)	24.66358(9)	24.67046(6)	24.67394(6)	24.67524(6)	24.67623(6)	24.67687(6)	24.67781(6)	24.67885(6)	24.67956(6)	24.67992(6)	24.68011(6)
Unit Cell Volume (Å)	15002.7(2)	15015.2(1)	15021.6(1)	15024.0(1)	15025.8(1)	15026.9(1)	15028.7(1)	15030.5(1)	15031.3(1)	15032.5(1)	15032.8(1)

Table 3 – Bond Distances (Å) and Angles (deg) in Dehydrated Li–A from 100–300 K (errors at 1σ level).

Bond Length/Angle	Temperature										
	300K	280K	260K	240K	220K	200K	180K	160K	140K	120K	100K
Si – O1	1.504(9)	1.504(9)	1.504(8)	1.504(9)	1.505(8)	1.504(8)	1.505(8)	1.505(8)	1.507(9)	1.507(9)	1.506(9)
Si – O2	1.587(7)	1.590(8)	1.591(8)	1.592(7)	1.593(7)	1.593(7)	1.592(7)	1.593(7)	1.593(8)	1.595(8)	1.595(8)
Si – O3	1.613(5)	1.616(5)	1.616(5)	1.615(5)	1.616(5)	1.615(5)	1.616(5)	1.616(5)	1.617(5)	1.619(5)	1.618(5)
Al – O1	1.791(9)	1.790(9)	1.791(9)	1.791(9)	1.791(8)	1.792(8)	1.792(8)	1.792(8)	1.790(9)	1.790(9)	1.790(9)
Al – O2	1.721(8)	1.723(8)	1.725(8)	1.726(8)	1.726(7)	1.726(7)	1.727(7)	1.727(7)	1.728(8)	1.727(8)	1.729(8)
Al – O3	1.766(5)	1.764(5)	1.765(5)	1.764(5)	1.763(5)	1.764(4)	1.763(5)	1.763(5)	1.763(5)	1.764(5)	1.765(5)
Si – O1 – Al	170.9(3)	170.8(3)	170.7(3)	170.7(3)	170.7(3)	170.7(3)	170.8(3)	170.8(3)	170.8(3)	170.8(3)	170.9(3)
Si – O2 – Al	133.0(5)	132.7(5)	132.5(5)	132.4(5)	132.4(4)	132.3(4)	132.3(4)	132.3(4)	132.1(5)	132.0(5)	131.9(5)
Si – O3 – Al	132.1(3)	132.0(3)	131.9(3)	131.9(3)	131.8(3)	131.8(3)	131.8(3)	131.8(3)	131.8(3)	131.6(3)	131.6(3)
O1 – Si – O2	107.8(4)	107.6(4)	107.5(4)	107.4(4)	107.4(4)	107.4(4)	107.4(4)	107.4(4)	107.3(4)	107.2(4)	107.1(4)
O1 – Si – O3	111.3(2)	111.2(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)
O2 – Si – O3	109.1(3)	109.1(3)	109.1(3)	109.1(3)	109.1(3)	109.1(2)	109.1(3)	109.1(3)	109.2(3)	109.1(3)	109.1(3)
O3 – Si – O3	108.4(4)	108.6(4)	108.8(4)	108.9(4)	108.9(4)	109.0(0)	108.9(4)	109.0(4)	109.0(4)	109.1(4)	109.2(4)
O1 – Al – O2	106.0(3)	105.9(3)	105.8(3)	105.7(3)	105.7(3)	105.7(3)	105.7(3)	105.7(3)	105.7(3)	105.6(3)	105.7(3)
O1 – Al – O3	111.4(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)	111.5(2)
O2 – Al – O3	108.6(3)	108.6(3)	108.5(2)	108.5(2)	108.5(2)	108.5(2)	108.5(2)	108.5(2)	108.5(2)	108.4(3)	108.4(2)
O3 – Al – O3	110.5(4)	110.7(4)	110.9(4)	110.9(3)	111.0(3)	111.0(3)	111.0(3)	111.0(3)	111.1(4)	111.1(4)	111.1(4)
Lattice Parameter (Å)	23.8806(3)	23.8806(1)	23.8806(1)	23.8800(1)	23.8798(1)	23.8797(1)	23.8797(1)	23.8800(1)	23.8804(1)	23.8807(1)	23.8809(1)
Unit Cell Volume (Å)	13618.6(6)	13618.7(2)	13618.6(2)	13617.7(2)	13617.2(2)	13617.2(2)	13617.1(2)	13617.6(2)	13618.4(2)	13618.9(2)	13619.2(1)

Table 4 *– Bond Distances (Å) and Angles (deg) in Dehydrated Na–A from 100–300 K (errors at 1σ level).*

Bond Length/Angle	Temperature										
	300K	280K	260K	240K	220K	200K	180K	160K	140K	120K	100K
Si – O1	1.503(7)	1.501(6)	1.499(6)	1.497(7)	1.493(7)	1.495(7)	1.498(7)	1.500(7)	1.502(8)	1.509(8)	1.511(8)
Si – O2	1.650(7)	1.652(7)	1.655(7)	1.661(7)	1.655(7)	1.657(7)	1.656(7)	1.652(7)	1.651(8)	1.646(8)	1.640(8)
Si – O3	1.587(5)	1.585(5)	1.583(5)	1.581(5)	1.576(5)	1.569(5)	1.565(5)	1.565(5)	1.565(5)	1.567(5)	1.571(5)
Al – O1	1.820(7)	1.825(7)	1.830(7)	1.838(7)	1.848(7)	1.858(7)	1.862(8)	1.860(8)	1.860(8)	1.854(8)	1.847(8)
Al – O2	1.649(7)	1.647(7)	1.646(7)	1.644(7)	1.649(7)	1.659(7)	1.669(8)	1.675(7)	1.679(8)	1.684(8)	1.687(8)
Al – O3	1.748(5)	1.749(5)	1.747(5)	1.745(5)	1.747(5)	1.740(5)	1.738(5)	1.738(5)	1.736(5)	1.737(5)	1.738(5)
Si – O1 – Al	143.0(3)	142.8(3)	142.8(3)	142.6(3)	142.0(3)	141.2(3)	140.4(3)	140.2(3)	140.0(4)	140.0(4)	140.1(4)
Si – O2 – Al	163.7(4)	163.4(4)	163.4(4)	162.7(4)	162.3(4)	161.8(4)	161.5(5)	161.4(4)	161.5(5)	161.3(5)	161.6(5)
Si – O3 – Al	146.0(3)	146.1(3)	146.1(3)	146.2(3)	146.8(3)	147.0(3)	147.0(3)	146.9(3)	146.9(3)	146.8(3)	146.6(3)
O1 – Si – O2	106.3(4)	106.1(4)	105.8(4)	105.4(4)	104.8(4)	104.3(4)	103.8(4)	108.6(3)	103.8(4)	103.9(4)	104.2(4)
O1 – Si – O3	112.4(3)	112.5(3)	112.7(3)	113.1(3)	114.2(3)	114.9(2)	115.2(2)	115.3(2)	115.3(2)	115.2(2)	115.1(2)
O2 – Si – O3	107.4(2)	107.6(21)	107.6(2)	107.8(2)	108.3(2)	108.6(2)	108.7(3)	103.8(4)	105.0(4)	108.7(2)	108.5(3)
O3 – Si – O3	110.6(2)	110.4(2)	110.0(2)	109.3(2)	106.9(2)	105.4(4)	105.1(4)	104.4(4)	108.6(3)	105.0(4)	105.1(4)
O1 – Al – O2	110.4(3)	110.3(3)	110.4(4)	109.9(4)	109.5(4)	108.7(4)	108.0(4)	107.8(4)	107.7(4)	107.4(4)	107.4(4)
O1 – Al – O3	111.4(2)	111.4(2)	111.6(2)	111.8(2)	112.6(2)	113.1(2)	113.4(2)	113.5(2)	113.5(2)	113.6(2)	113.6(2)
O2 – Al – O3	107.4(2)	107.6(2)	107.6(2)	107.9(2)	108.4(2)	108.7(2)	108.8(2)	108.8(2)	108.7(3)	108.7(3)	108.5(3)
O3 – Al – O3	108.8(4)	108.5(4)	107.9(4)	107.4(4)	105.3(4)	104.3(4)	104.3(4)	104.4(4)	104.5(4)	104.7(4)	105.0(4)
Lattice Parameter (Å)	24.55930(8)	24.55958(8)	24.55995(8)	24.56104(9)	24.56310(9)	24.56459(9)	24.56557(9)	24.56605(9)	24.56723(9)	24.56818(9)	24.56898(9)
Unit Cell Volume (Å)	14813.2(2)	14813.7(2)	14814.3(2)	14816.3(2)	14820.0(2)	14822.7(2)	14824.5(2)	14825.4(2)	14827.5 (2)	14829.2(2)	14830.7(2)

Table 5 – Bond Distances (Å) and Angles (deg) in Dehydrated K–A from 100–300 K (errors at 1σ level).

Bond Length/Angle	Temperature										
	300K	280K	260K	240K	220K	200K	180K	160K	140K	120K	100K
Si – O1	1.52(1)	1.53(1)	1.52(1)	1.52(1)	1.52(1)	1.52(1)	1.52(1)	1.51(1)	1.52(1)	1.51(2)	1.51(1)
Si – O2	1.57(1)	1.57(1)	1.58(1)	1.58(1)	1.59(1)	1.59(1)	1.59(1)	1.59(1)	1.60(1)	1.60(2)	1.60(1)
Si – O3	1.584(9)	1.584(8)	1.586(8)	1.586(8)	1.585(7)	1.585(7)	1.585(8)	1.585(8)	1.588(8)	1.59(1)	1.589(7)
Al – O1	1.76(1)	1.75(1)	1.76(1)	1.76(1)	1.77(1)	1.77(1)	1.77(1)	1.78(1)	1.77(1)	1.78(2)	1.78(1)
Al – O2	1.73(1)	1.73(1)	1.72(1)	1.72(1)	1.72(1)	1.72(1)	1.72(1)	1.71(1)	1.71(1)	1.71(2)	1.71(1)
Al – O3	1.764(9)	1.762(8)	1.758(8)	1.757(8)	1.756(7)	1.756(7)	1.754(8)	1.755(8)	1.754(8)	1.76(1)	1.753(7)
Si – O1 – Al	134.2(5)	134.0(5)	133.6(5)	133.6(4)	133.4(4)	133.4(4)	132.8(5)	132.8(5)	132.6(4)	132.6(6)	131.7(4)
Si – O2 – Al	175.6(9)	175.9(8)	176.5(8)	176.5(8)	176.4(7)	176.7(8)	176.5(9)	176.7(8)	177.2(8)	177.3(9)	177.8(7)
Si – O3 – Al	152.4(5)	152.5(5)	152.5(5)	152.5(5)	152.6(4)	152.7(5)	152.8(5)	152.8(5)	152.7(5)	152.9(6)	153.1(4)
O1 – Si – O2	109.1(7)	109.3(7)	109.7(6)	109.7(6)	109.7(6)	109.9(6)	109.6(7)	109.8(6)	110.1(6)	110.1(8)	110.1(5)
O1 – Si – O3	111.9(4)	111.8(3)	111.9(3)	111.8(3)	111.8(3)	111.7(3)	111.7(4)	111.8(4)	111.7(3)	111.7(4)	111.6(3)
O2 – Si – O3	107.5(4)	107.4(4)	107.2(4)	107.2(4)	107.2(3)	107.2(4)	107.3(4)	107.3(4)	107.1(4)	107.2(5)	107.2(3)
O3 – Si – O3	108.9(7)	108.9(7)	108.9(6)	108.9(6)	109.0(6)	108.8(6)	108.9(7)	108.8(6)	109.0(6)	108.9(8)	108.9(5)
O1 – Al – O2	110.7(7)	110.6(6)	110.5(6)	110.4(6)	110.1(5)	110.1(5)	109.6(6)	109.7(6)	109.7(5)	109.8(7)	109.5(5)
O1 – Al – O3	110.8(3)	110.7(3)	110.5(3)	110.4(3)	110.3(3)	110.3(3)	110.3(3)	110.2(3)	110.2(3)	110.1(4)	110.1(3)
O2 – Al – O3	107.9(4)	107.9(4)	107.9(4)	108.0(3)	108.1(3)	108.1(3)	108.2(4)	108.2(4)	108.1(3)	108.1(5)	108.1(3)
O3 – Al – O3	108.7(6)	108.9(6)	109.4(6)	109.7(6)	109.9(5)	109.9(5)	110.3(6)	110.4(6)	110.7(6)	110.6(7)	110.9(5)
Lattice Parameter (Å)	24.5583(2)	24.5582(1)	24.5581(1)	24.5579(1)	24.5575(1)	24.5571(4)	24.5572(2)	24.5570(2)	24.5567(2)	24.5569(2)	24.5581(1)
Unit Cell Volume (Å)	14811.3(3)	14811.1(3)	14810.9(3)	14810.6(2)	14809.9(2)	14809.2(3)	14809.3(3)	14809.0(3)	14808.5(3)	14808.7(4)	14810.9(3)

Table 6 – Bond Distances (Å) and Angles (deg) in Dehydrated $Rb_{0.79}Na_{0.21}$-A from 100–300 K (errors at 1σ level).

Bond Length/Angle	Temperature										
	300K	280K	260K	240K	220K	200K	180K	160K	140K	120K	100K
Si – O1	1.523(8)	1.521(8)	1.520(8)	1.519(8)	1.519(8)	1.516(8)	1.515(8)	1.513(8)	1.511(8)	1.515(8)	1.514(8)
Si – O2	1.594(8)	1.585(5)	1.592(7)	1.591(7)	1.590(7)	1.590(7)	1.590(8)	1.590(8)	1.588(7)	1.588(7)	1.588(8)
Si – O3	1.584(5)	1.585(5)	1.587(5)	1.588(5)	1.589(5)	1.590(5)	1.591(5)	1.593(5)	1.594(5)	1.596(5)	1.596(5)
Al – O1	1.779(9)	1.781(8)	1.782(8)	1.784(8)	1.783(8)	1.786(8)	1.787(8)	1.789(8)	1.791(8)	1.788(8)	1.790(8)
Al – O2	1.705(8)	1.705(8)	1.707(7)	1.708(7)	1.709(7)	1.710(8)	1.709(8)	1.708(8)	1.709(8)	1.711(8)	1.712(8)
Al – O3	1.751(5)	1.750(5)	1.749(5)	1.748(5)	1.748(5)	1.748(5)	1.747(5)	1.746(5)	1.745(5)	1.743(5)	1.741(5)
Si – O1 – Al	139.9(3)	139.8(3)	139.8(3)	139.7(3)	139.6(3)	139.5(3)	139.4(3)	139.4(3)	139.3(3)	139.2(3)	139.1(3)
Si – O2 – Al	166.9(5)	167.0(5)	167.1(5)	167.0(5)	167.1(5)	167.1(5)	167.1(5)	167.2(5)	167.2(5)	167.3(5)	167.3(5)
Si – O3 – Al	147.6(3)	147.6(3)	147.6(3)	147.6(3)	147.6(3)	147.6(3)	147.6(3)	147.7(3)	147.7(3)	147.7(3)	147.7(3)
O1 – Si – O2	108.1(4)	108.1(4)	108.1(4)	107.9(4)	107.9(3)	107.8(4)	107.7(4)	107.6(4)	107.6(4)	107.6(4)	107.5(4)
O1 – Si – O3	111.1(2)	111.1(2)	111.2(2)	111.1(2)	111.1(2)	111.2(2)	111.2(2)	111.2(2)	111.3(2)	111.3(2)	111.3(2)
O2 – Si – O3	107.8(2)	107.7(2)	107.7(2)	107.8(2)	107.8(2)	107.8(2)	107.9(2)	107.9(2)	107.9(2)	107.9(2)	107.9(2)
O3 – Si – O3	110.9(4)	110.9(4)	110.8(4)	110.9(4)	110.8(4)	110.9(4)	110.9(4)	110.8(4)	110.7(4)	110.8(4)	110.8(4)
O1 – Al – O2	108.7(4)	108.7(3)	108.8(3)	108.8(3)	108.8(3)	108.8(3)	108.9(4)	108.9(4)	109.0(4)	109.0(3)	109.0(4)
O1 – Al – O3	111.0(2)	111.0(2)	111.0(2)	111.0(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.1(2)	111.2(2)	111.2(2)
O2 – Al – O3	107.2(2)	107.2(2)	107.2(2)	107.2(2)	107.1(2)	107.1(2)	107.1(2)	107.1(3)	107.1(2)	107.0(2)	107.0(2)
O3 – Al – O3	111.6(4)	111.6(4)	111.6(3)	111.5(3)	111.5(3)	111.5(3)	111.4(4)	111.4(4)	111.3(4)	111.4(4)	111.3(4)
Lattice Parameter (Å)	24.53332(4)	24.53393(4)	24.53429(4)	24.53471(4)	24.53488(4)	24.53495(4)	24.53513(4)	24.53502(4)	24.53501(4)	24.53493(4)	24.53467(4)
Unit Cell Volume (Å)	14766.21(7)	14767.31(7)	14767.97(7)	14768.71(7)	14769.03(7)	14769.16(7)	14769.49(7)	14769.28(7)	14769.25(7)	14769.12(7)	14768.65(7)

Table 7 – Bond Distances (Å) and Angles (deg) in Dehydrated $Cs_{0.58}Na_{0.42}$-A from 100–300 K (errors at 1σ level).

Bond Length/Angle	Temperature										
	300K	280K	260K	240K	220K	200K	180K	160K	140K	120K	100K
Si – O1	1.50(1)	1.50(9)	1.50(9)	1.50(9)	1.49(9)	1.49(9)	1.49(9)	1.50(1)	1.50(9)	1.50(9)	1.50(1)
Si – O2	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)	1.60(1)
Si – O3	1.610(8)	1.611(7)	1.611(7)	1.611(7)	1.611(7)	1.612(7)	1.613(7)	1.614(8)	1.613(7)	1.614(7)	1.615(8)
Al – O1	1.83(1)	1.829(9)	1.830(9)	1.830(9)	1.831(9)	1.832(9)	1.833(9)	1.83(1)	1.83(1)	1.835(9)	1.84(1)
Al – O2	1.71(1)	1.71(1)	1.71(1)	1.71(1)	1.71(1)	1.71(1)	1.71(1)	1.71(1)	1.72(1)	1.71(1)	1.71(1)
Al – O3	1.729(8)	1.728(7)	1.728(7)	1.728(7)	1.729(7)	1.728(7)	1.728(7)	1.729(8)	1.730(8)	1.729(8)	1.730(8)
Si – O1 – Al	148.8(5)	148.8(5)	148.9(5)	148.9(5)	148.9(5)	148.9(4)	149.0(4)	149.0(5)	149.0(5)	149.0(5)	148.9(5)
Si – O2 – Al	157.9(8)	157.8(7)	157.7(7)	157.7(7)	157.6(7)	157.7(7)	157.7(7)	157.7(8)	157.7(7)	157.8(7)	158.0(8)
Si – O3 – Al	141.9(5)	141.9(4)	141.9(4)	141.9(4)	141.9(4)	141.9(4)	141.8(4)	141.7(5)	141.6(4)	141.6(4)	141.5(5)
O1 – Si – O2	106.6(7)	106.6(6)	106.6(6)	106.6(6)	106.6(6)	106.6(6)	106.7(6)	106.6(7)	106.6(6)	106.6(6)	106.7(7)
O1 – Si – O3	112.2(3)	112.2(3)	112.2(3)	112.2(3)	112.2(3)	112.2(3)	112.2(3)	112.2(3)	112.2(3)	112.3(3)	112.3(3)
O2 – Si – O3	107.5(4)	107.5(3)	107.5(3)	107.5(3)	107.5(3)	107.5(3)	107.5(3)	107.4(4)	107.4(4)	107.3(4)	107.2(4)
O3 – Si – O3	110.6(6)	110.5(5)	110.6(6)	110.6(6)	110.6(6)	110.6(5)	110.6(5)	110.8(6)	110.7(6)	110.8(6)	110.8(6)
O1 – Al – O2	110.0(6)	110.0(5)	110.0(5)	110.0(5)	110.0(5)	110.0(5)	110.1(5)	110.1(6)	110.1(6)	110.1(5)	110.2(6)
O1 – Al – O3	111.9(3)	111.9(2)	111.9(3)	111.9(3)	111.9(3)	111.9(2)	111.9(2)	111.9(3)	111.9(3)	111.9(3)	111.9(3)
O2 – Al – O3	106.4(4)	106.4(3)	106.4(3)	106.4(3)	106.4(3)	106.4(3)	106.4(3)	106.3(4)	106.3(3)	106.3(3)	106.2(4)
O3 – Al – O3	110.0(6)	109.9(5)	110.0(5)	110.0(5)	110.0(5)	110.0(5)	110.0(5)	110.1(6)	110.1(6)	110.2(5)	110.2(6)
Lattice Parameter (Å)	24.49934(7)	24.4999(6)	24.50034(6)	24.50077(6)	24.50114(6)	24.50174(6)	24.50195(6)	24.50261(7)	24.50233(7)	24.50236(6)	24.50199(7)
Unit Cell Volume (Å)	14704.9(1)	14705.9(1)	14706.7(1)	14707.5(1)	14708.2(1)	14709.3(1)	14709.6(1)	14710.8(1)	14710.3(1)	14710.4(1)	14709.7(1)

Unit Cell Volume and Bond Angle Graphs

ITQ–29

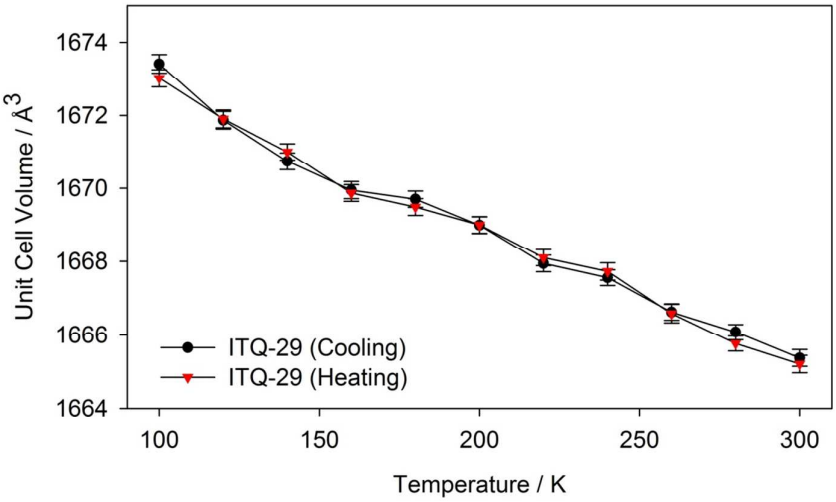

Figure 1 – Calculated unit cell volumes of ITQ-29 from 100–300 K.

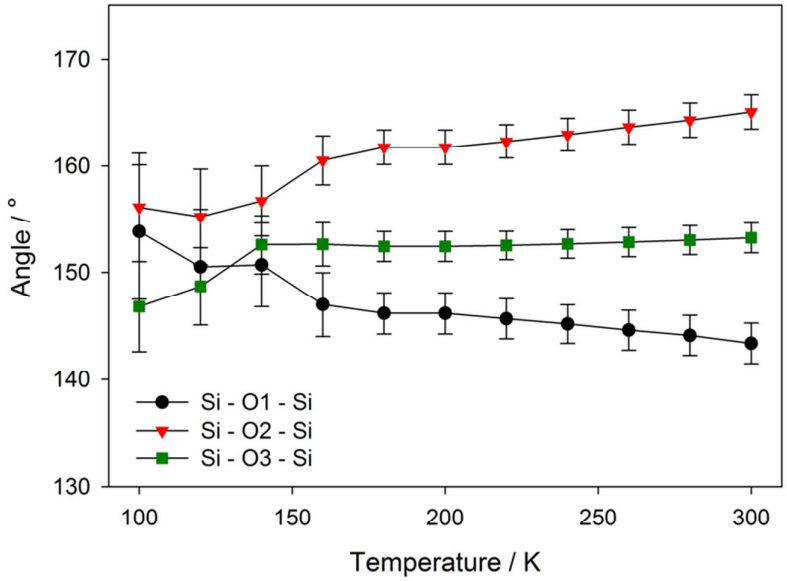

Figure 2 – Calculated Si–O–Si bond angles for ITQ-29 from 100–300 K.

Dehydrated Ag-A

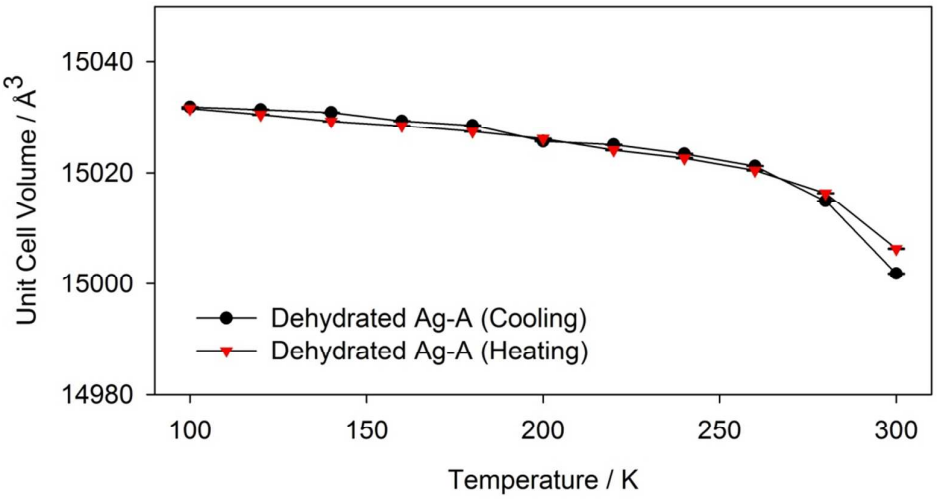

Figure 3 – Calculated unit cell volumes of dehydrated Ag-A from 100–300 K.

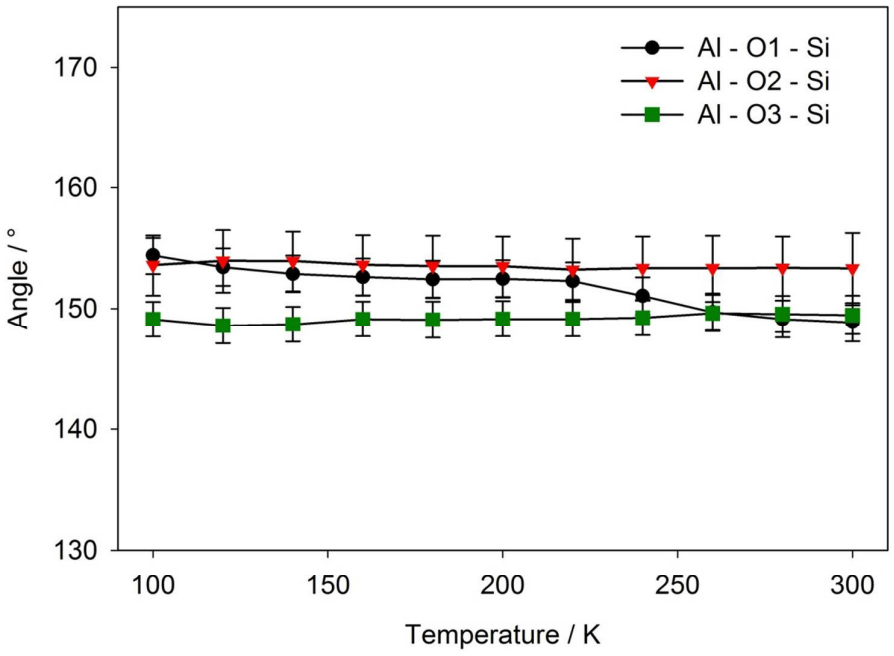

Figure 4 – Calculated Si–O–Al bond angles for dehydrated Ag-A from 100–300 K.

Dehydrated Li-A

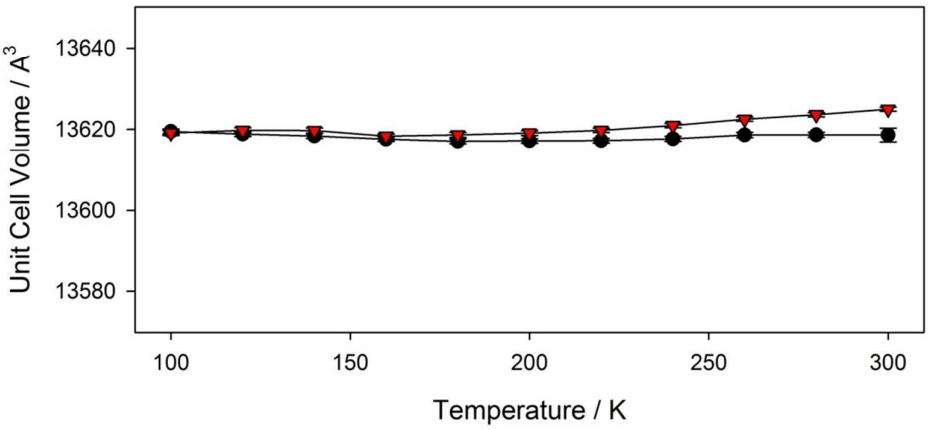

Figure 5 – Calculated unit cell volumes of dehydrated Li-A from 100–300 K.

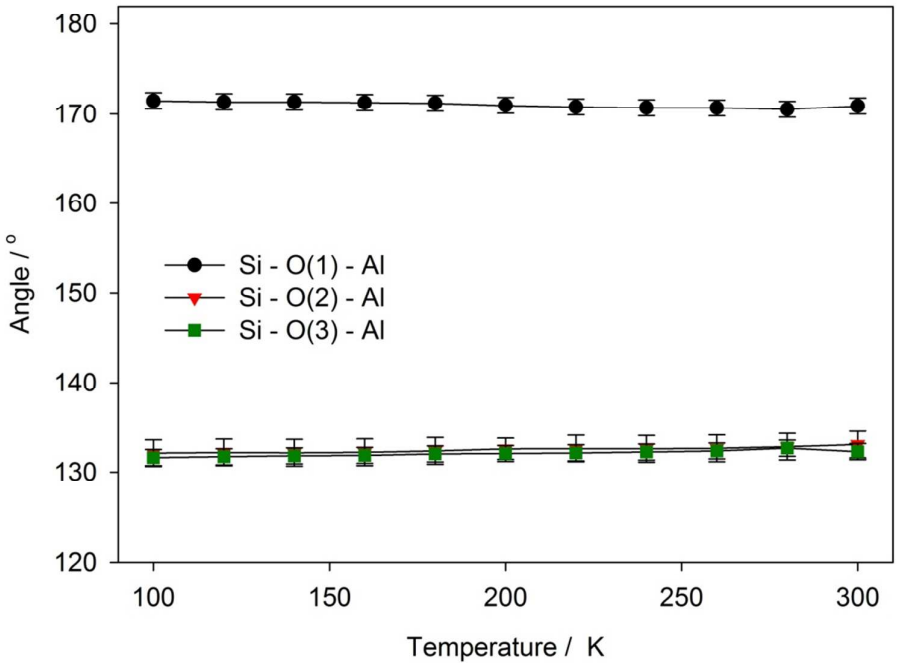

Figure 6 – Calculated Si–O–Al bond angles for dehydrated Li-A from 100–300 K.

Dehydrated K-A

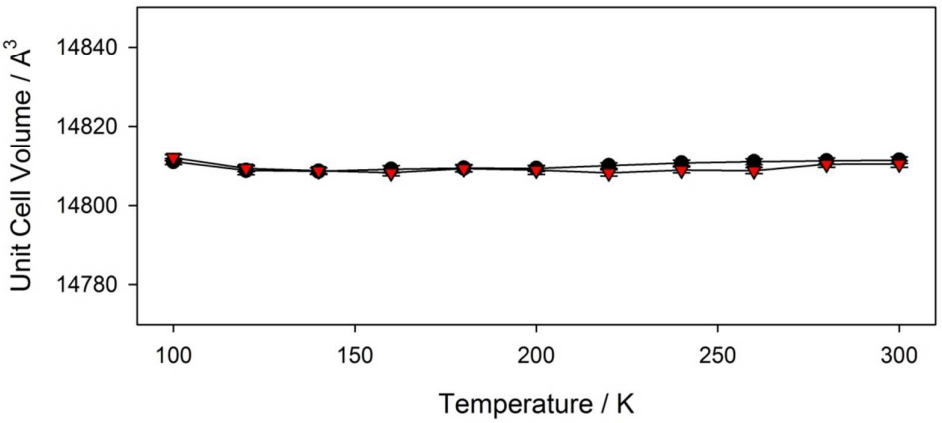

Figure 7 – Calculated unit cell volumes of dehydrated K-A from 100–300 K.

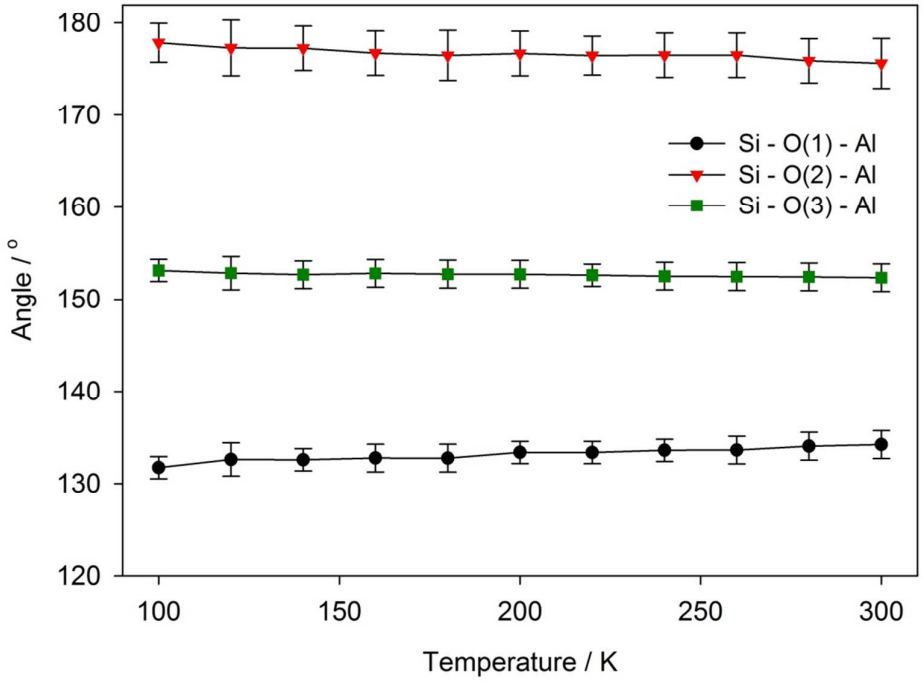

Figure 8 – Calculated Si–O–Al bond angles for dehydrated K-A from 100–300 K.

Dehydrated $Rb_{0.79}Na_{0.21}$-A

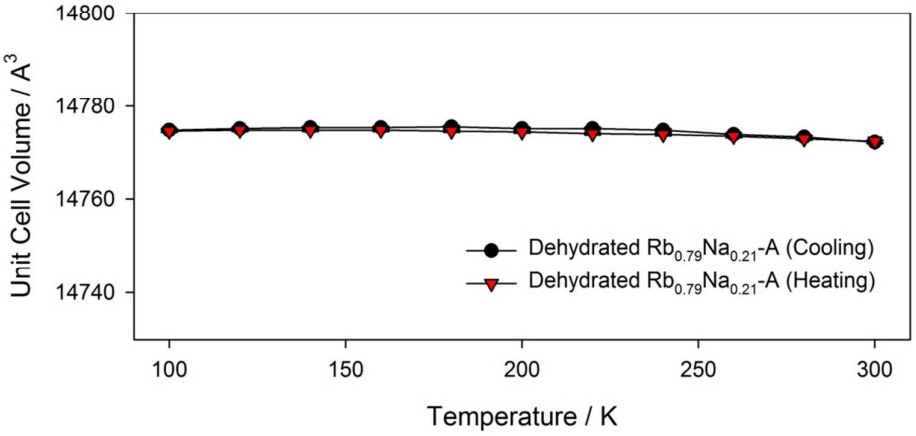

Figure 9 – Calculated unit cell volumes of dehydrated $Rb_{0.79}Na_{0.21}$-A from 100–300 K.

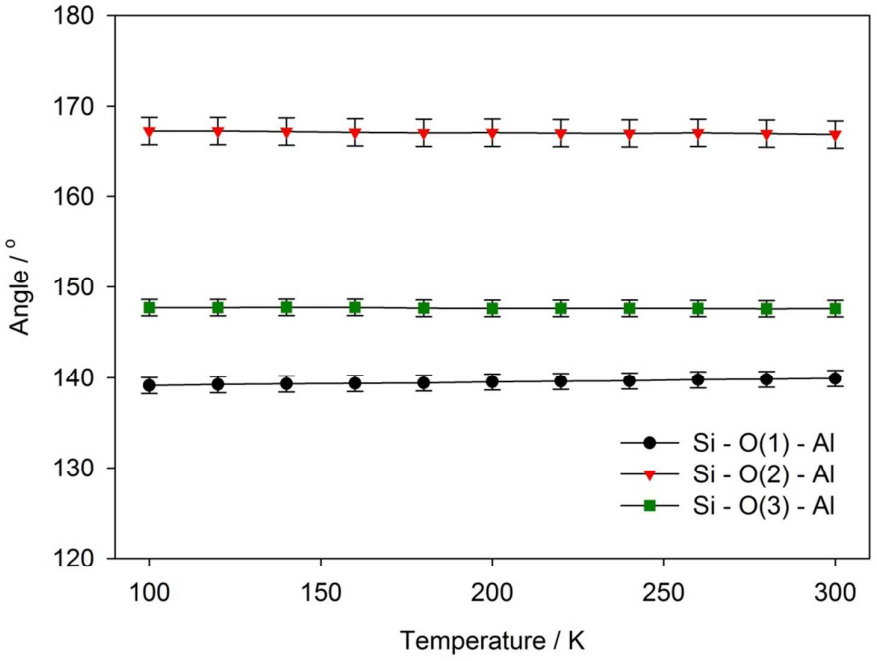

Figure 10 – Calculated Si–O–Al bond angles for dehydrated $Rb_{0.79}Na_{0.21}$-A from 100–300 K.

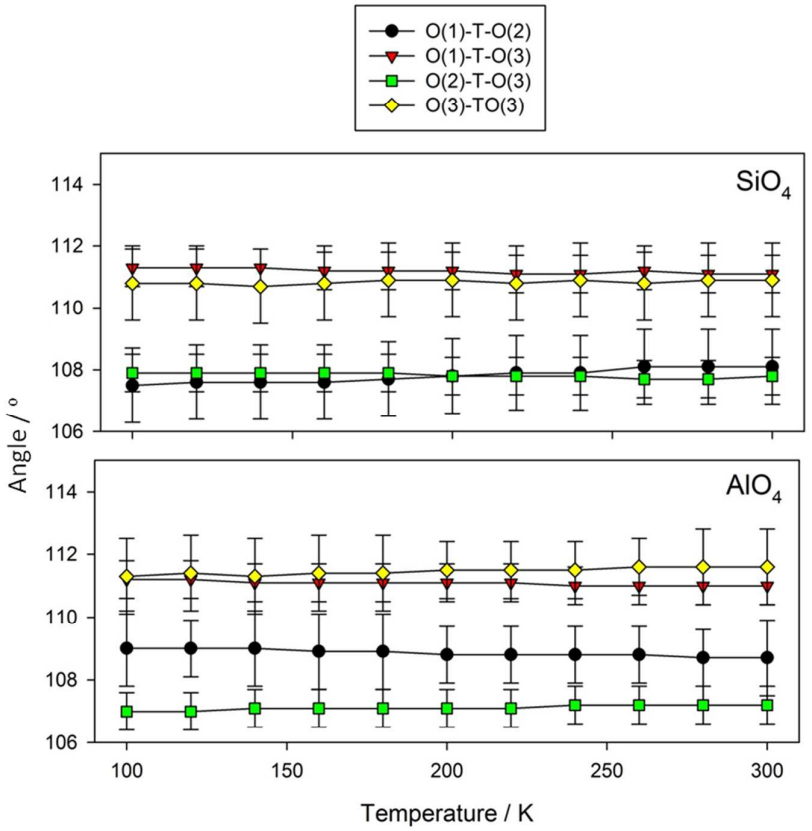

Figure 11 - Calculated O-T-O bond angles for dehydrated $Rb_{0.79}Na_{0.21}$-A from 100–300 K.

Dehydrated $Cs_{0.58}Na_{0.42}$-A

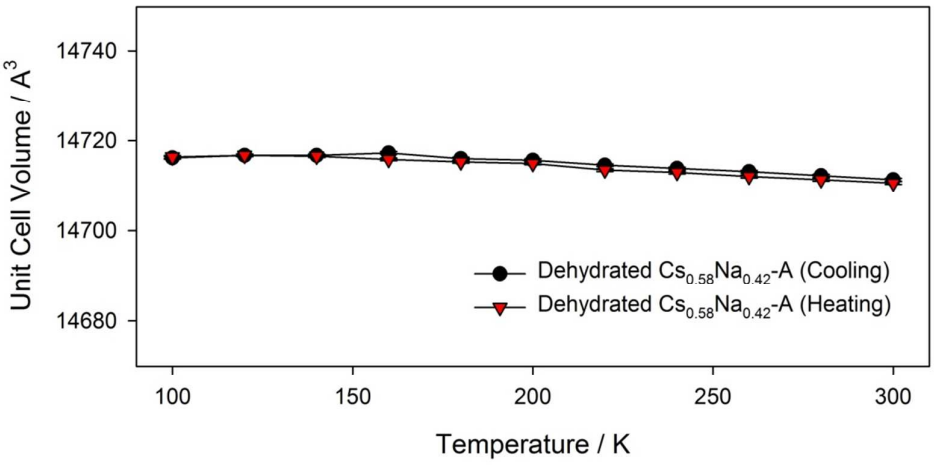

Figure 12 – Calculated unit cell volumes of dehydrated $Cs_{0.58}Na_{0.42}$-A from 100–300 K.

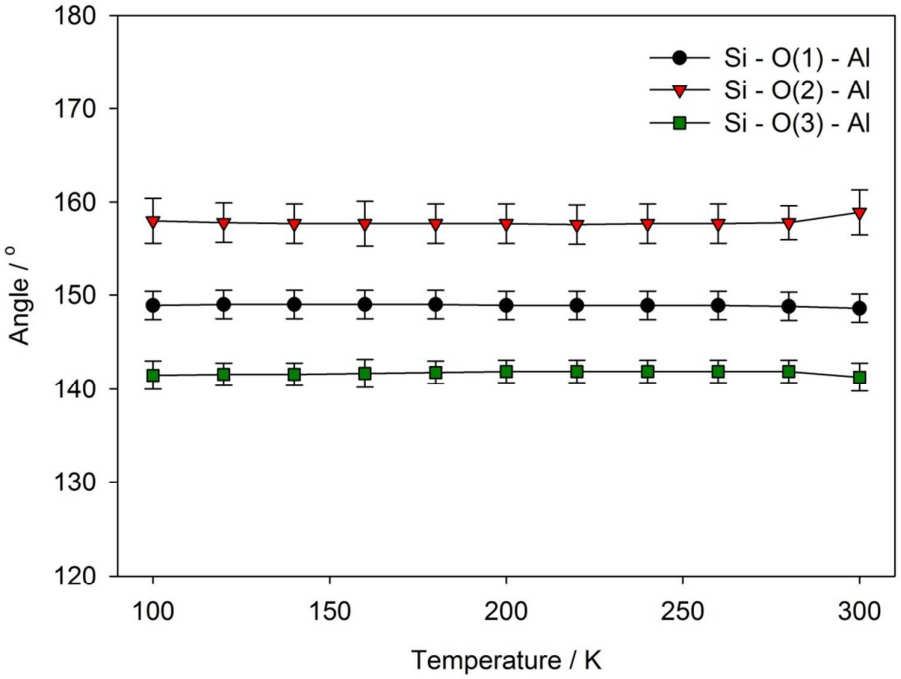

Figure 13 – Calculated Si–O–Al bond angles for dehydrated $Cs_{0.58}Na_{0.42}$-A from 100–300 K.

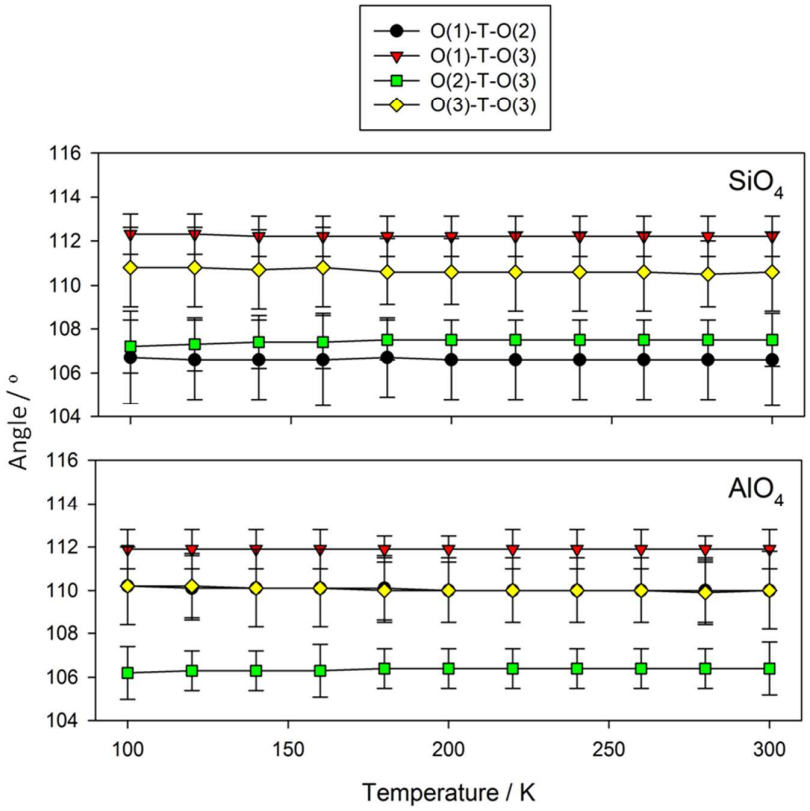

Figure 14 - Calculated O-T-O bond angles for dehydrated $Cs_{0.58}Na_{0.42}$-A from 100–300 K.

Rietveld Refinement Tables

Table 8 – *Refined atomic parameters of ITQ-29 at 300 K.*

Atom	Wyckoff position	*x*	*y*	*z*	Occupancy	B
Si(1)	24k	0	0.3701(3)	0.1840(3)	1	1.4(1)
O(1)	12h	0	0.5	0.2235(7)	1	1.7(1)
O(2)	12i	0	0.2913(4)	0.2913(4)	1	1.7(1)
O(3)	24m	0.1086(3)	0.1086(3)	0.3481(4)	1	1.7(1)

[a] *a* = 11.853(2)*) Å, space group:* $Pm\bar{3}m$, $\chi^2 = 1.59$, $R_{wp} = 7.29$ %, $R_p = 4.58$ %.

Table 9 *– Refined atomic parameters of dehydrated Ag-A at 300 K.*

Atom	Wyckoff Position	*x*	*y*	*z*	Occupancy	B
Si(1)	96i	0	0.0939(3)	0.1841(3)	1	0.70(4)
Al(1)	96i	0	0.1853(3)	0.0914(3)	1	0.70(4)
O(1)	96i	0	0.1109(2)	0.2479(7)	1	1.38(9)
O(2)	96i	0	0.1476(6)	0.1515(6)	1	1.38(9)
O(3)	192j	0.0529(3)	0.0568(3)	0.1714(2)	1	1.38(9)
Ag(1)	64g	0.0964(3)	0.0964(3)	0.0964(3)	0.97(3)	2.90(4)
Ag(2)	96i	0	0.2227(2)	0.2089(3)	0.19(1)	2.90(4)
Ag(3)	48e	0	0	0.0806(3)	0.17(2)	2.90(4)

[a] *a* = 24.66358(7) *Å, space group:* $Fm\bar{3}c$, $\chi^2 = 1.30$, $R_{wp} = 8.89$ %, $R_p = 6.84$ %.

Table 10 *– Refined atomic parameters of dehydrated Li-A at 300K*[a]

	Atom	Wyckoff position	*x*	*y*	*z*	Occupancy	B
Framework	Si(1)	96i	0	0.0932(2)	0.1806(2)	1	0.90(4)
	Al(1)	96i	0	0.1818(2)	0.0896(2)	1	0.90(4)
	O(1)	96i	0	0.0970(2)	0.2436(3)	1	0.69(6)
	O(2)	96i	0	0.1552(3)	0.1566(3)	1	0.69(6)
	O(3)	192j	0.0548(2)	0.0608(2)	0.1581(1)	1	0.69(6)
6R	Ag(1)	64g	0.0980(4)	0.0980(4)	0.0980(4)	0.84(3)	0.3(5)
8R	Ag(2)	96i	0	0.232(9)	0.234(9)	0.25(1)	0.3(5)

[a] *a = 23.88056(8) Å, space group:* $Fm\bar{3}c$, $\chi^2 = 2.52$, $R_{wp} = 19.58$ %, $R_p = 12.32$ %.

Figure 11 *– Refined atomic parameters of dehydrated Na-A at 300K*[a]

	Atom	Wyckoff position	*x*	*y*	*z*	Occupancy	B
Framework	Si(1)	96i	0	0.0920(2)	0.1849(1)	1	1.34(2)
	Al(1)	96i	0	0.1867(2)	0.0916(2)	1	1.34(2)
	O(1)	96i	0	0.1131(1)	0.2424(2)	1	1.79(4)
	O(2)	96i	0	0.1460(2)	0.1450(2)	1	1.79(4)
	O(3)	192j	0.0531(2)	0.0579(2)	0.1713(1)	1	1.79(4)
6R	Na(1)	64g	0.5992(1)	0.5992(1)	0.5992(1)	0.965(5)	2.0(1)
8R	Na(2)	96i	0	0.2779(6)	0.2119(6)	0.189(2)	2.0(1)

[a] *a = 24.55930(8) Å, space group: $Fm\bar{3}c$, χ^2 = 1.40, R_{wp} = 14.17 %, R_p = 11.96 %.*

Figure 12 – Refined atomic parameters of dehydrated K-A at 300K[a]

	Atom	Wyckoff position	x	y	z	Occupancy	B
Framework	Si(1)	96i	0	0.0944(4)	0.1881(3)	1	0.49(4)
	Al(1)	96i	0	0.1889(3)	0.0928(4)	1	0.49(4)
	O(1)	96i	0	0.1195(2)	0.2448(5)	1	1.35(7)
	O(2)	96i	0	0.1411(5)	0.1447(4)	1	1.35(7)
	O(3)	192j	0.0525(3)	0.0584(3)	0.1777(1)	1	1.35(7)
6R	K(1)	64g	0.1158(1)	0.1158(1)	0.1158(1)	0.868(5)	3.4(1)
	K(2)	64g	0.0716(4)	0.0716(4)	0.0716(4)	0.152(3)	3.4(1)
8R	K(3)	96i	0	0.240(4)	0.236(2)	0.236(2)	3.4(1)

[a] *a = 24.55825(15) Å, space group: $Fm\bar{3}c$, χ^2 = 2.67, R_{wp} = 21.90 %, R_p = 13.40 %.*

Table 13 *– Refined atomic parameters of dehydrated $Rb_{0.79}Na_{0.21}$-A at 300K*[a]

	Atom	Wyckoff position	x	y	z	Occupancy	B
Framework	Si(1)	96i	0	0.0936(2)	0.1858(2)	1	1.15(3)
	Al(1)	96i	0	0.1876(2)	0.0910(2)	1	1.15(3)
	O(1)	96i	0	0.1153(1)	0.2441(3)	1	1.87(5)
	O(2)	96i	0	0.1445(3)	0.1455(3)	1	1.87(5)
	O(3)	192j	0.0532(2)	0.0590(2)	0.1739(1)	1	1.87(5)
6R	Na(1)	64g	0.1011(2)	0.1011(2)	0.1011(2)	0.527(2)	0.4(2)
	Rb(1)	64g	0.1274(1)	0.1274(1)	0.1274(1)	0.447(7)	3.52(6)
	Rb(2)	64g	0.0489(2)	0.0489(2)	0.0489(2)	0.118(8)	3.52(6)
8R	Rb(3)	96i	0	0.250(4)	0.234(2)	0.248(5)	3.52(6)

[a] *a = 24.55332(4) Å, space group: $Fm\bar{3}c$, χ^2 = 1.74, R_{wp} = 13.06 %, R_p = 9.91 %.*

Table 14 *– Refined atomic parameters of dehydrated $Cs_{0.58}Na0_{0.42}$-A at 300K*[a]

	Atom	Wyckoff position	x	y	z	Occupancy	B
Framework	Si(1)	96i	0	0.0917(3)	0.1842(2)	1	1.03(4)
	Al(1)	96i	0	0.1861(3)	0.0905(3)	1	1.03(4)
	O(1)	96i	0	0.1092(2)	0.2413(4)	1	1.65(7)
	O(2)	96i	0	0.1459(4)	0.1478(4)	1	1.65(7)
	O(3)	192j	0.0543(3)	0.0580(3)	0.1682(1)	1	1.65(7)
6R	Na(1)	64g	0.1009(1)	0.1009(1)	0.1009(1)	0.679(8)	0.9(8)
	Cs(1)	64g	0.0406(2)	0.0406(2)	0.0406(2)	0.107(6)	5.8(8)
	Cs(2)	64g	0.1385(1)	0.1385(1)	0.1385(1)	0.171(2)	5.8(8)
8R	Cs(3)	96i	0	0.2600(5)	0.2502(1)	0.253(5)	5.8(8)

[a] *$a = 24.49934(7)$ Å, space group: $Fm\bar{3}c$, $\chi^2 = 2.63$, $R_{wp} = 16.48\%$, $R_p = 10.15\%$.*

Rietveld Refinement Plots

ITQ-29

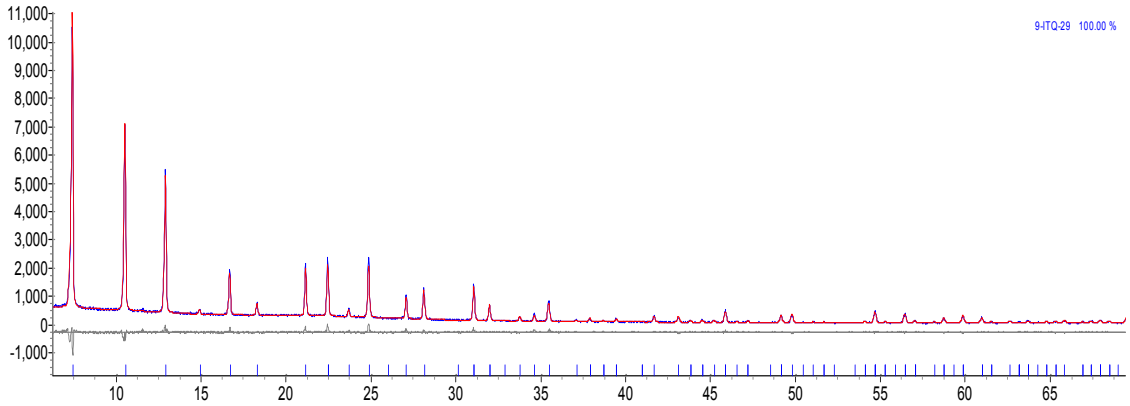

Figure 15 - Rietveld refinement plot of ITQ-29 at 300 K.

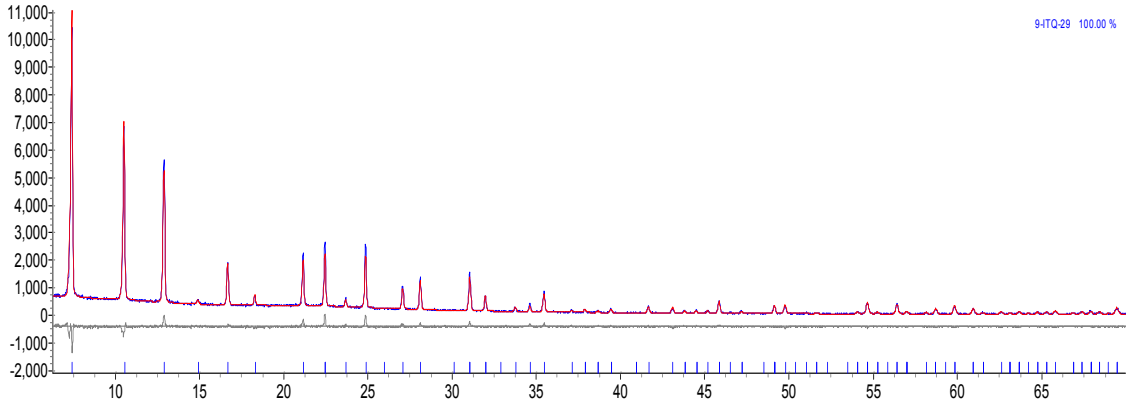

Figure 16 - Rietveld refinement plot of ITQ-29 at 200 K.

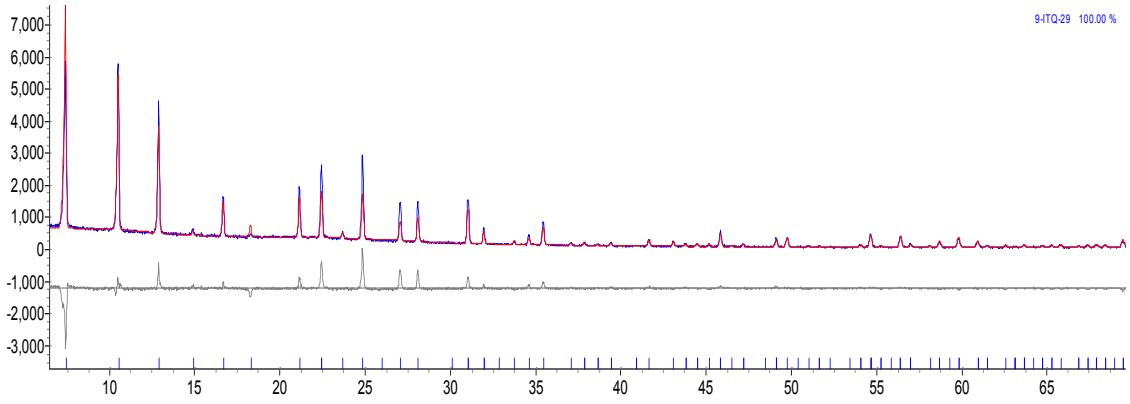

Figure 17 - Rietveld refinement plot of ITQ-29 at 100 K.

Dehydrated Ag-A

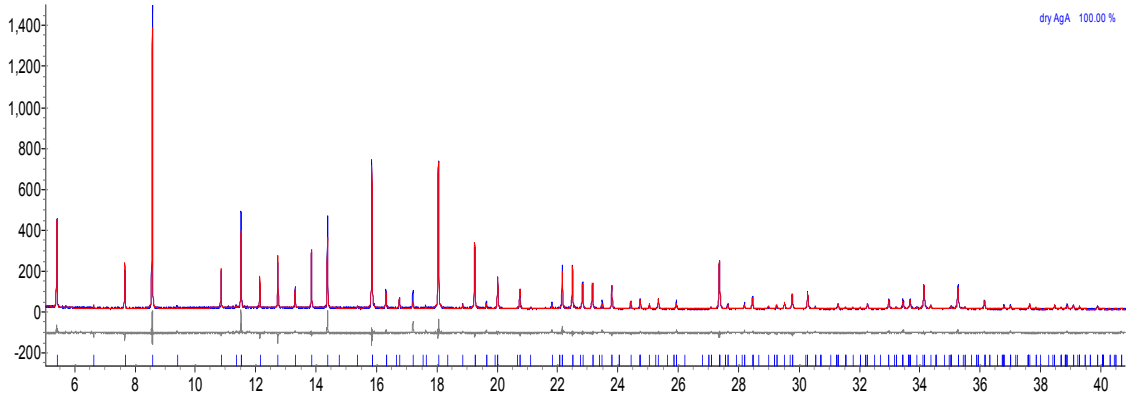

Figure 18 - Rietveld refinement plot of dehydrated Ag-A at 300 K.

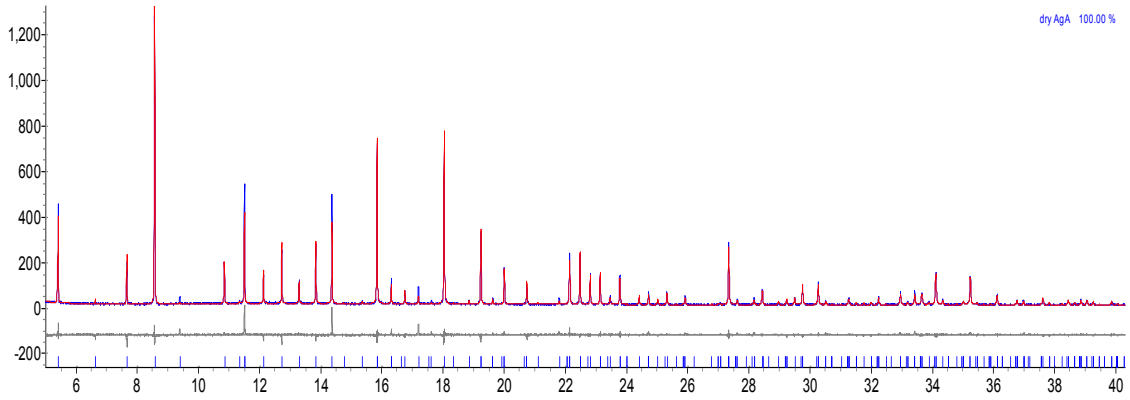

Figure 19 - Rietveld refinement plot of dehydrated Ag-A at 200 K.

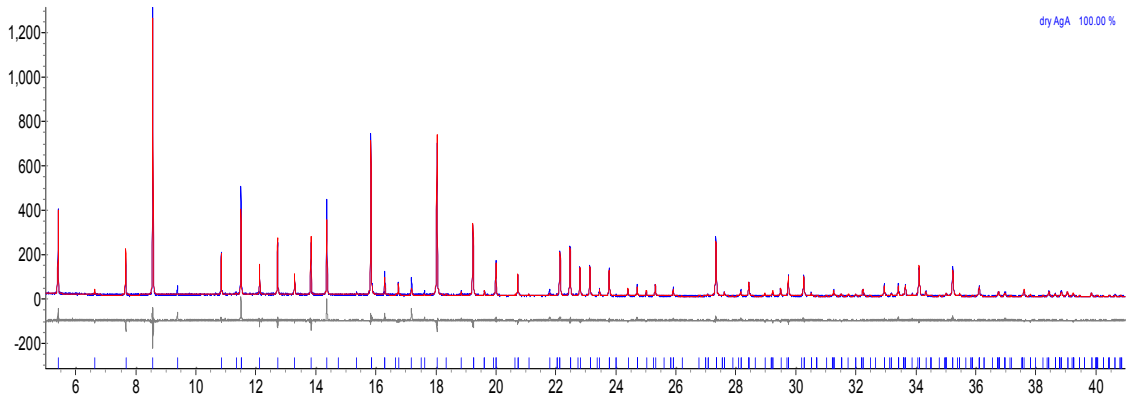

Figure 20 - Rietveld refinement plot of dehydrated Ag-A at 100 K.

Dehydrated Li-A

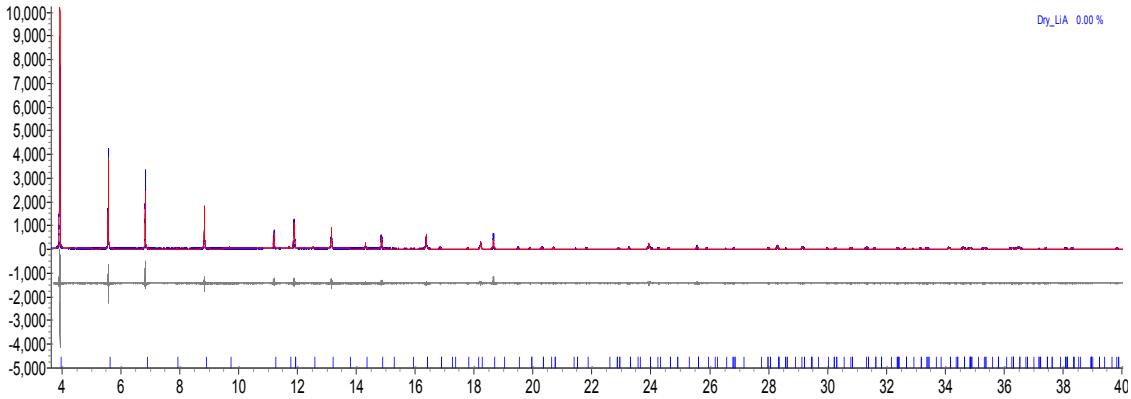

Figure 21 - Rietveld refinement plot of dehydrated Li-A at 300 K.

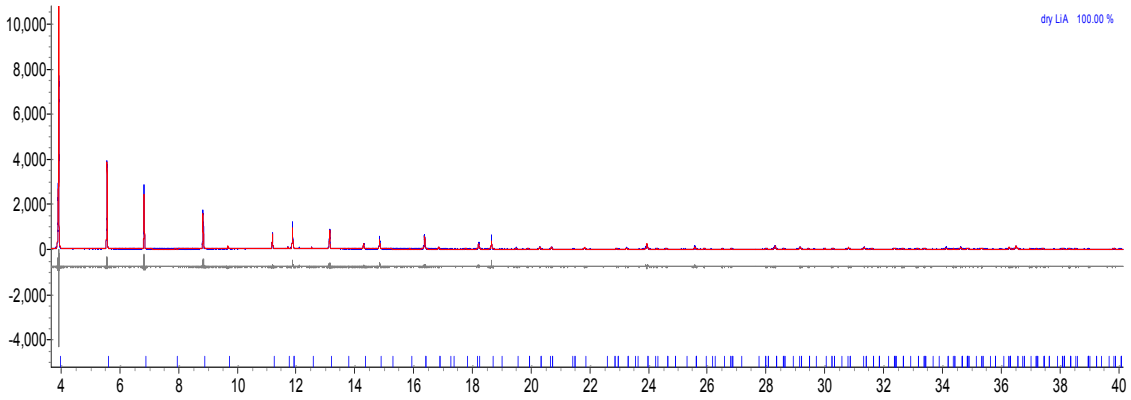

Figure 22 - Rietveld refinement plot of dehydrated LI-A at 200 K.

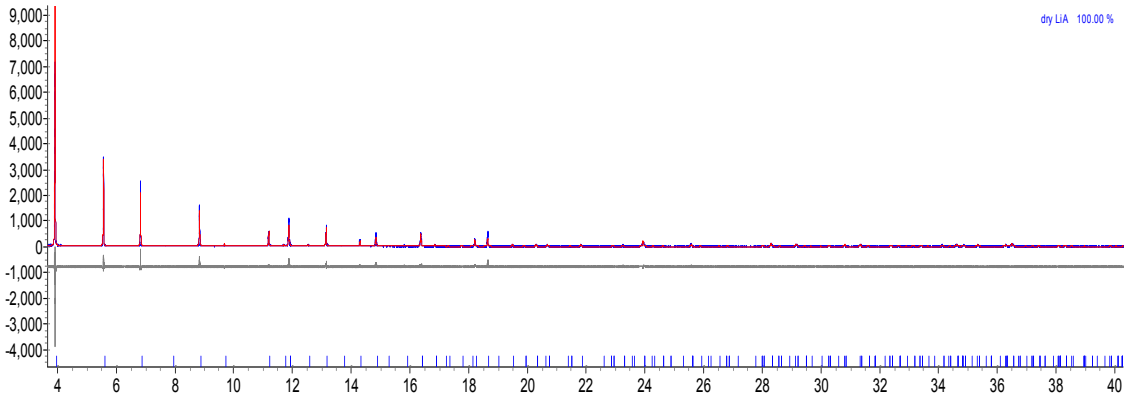

Figure 23 - Rietveld refinement plot of dehydrated Li-A at 100 K.

Dehydrated Na-A

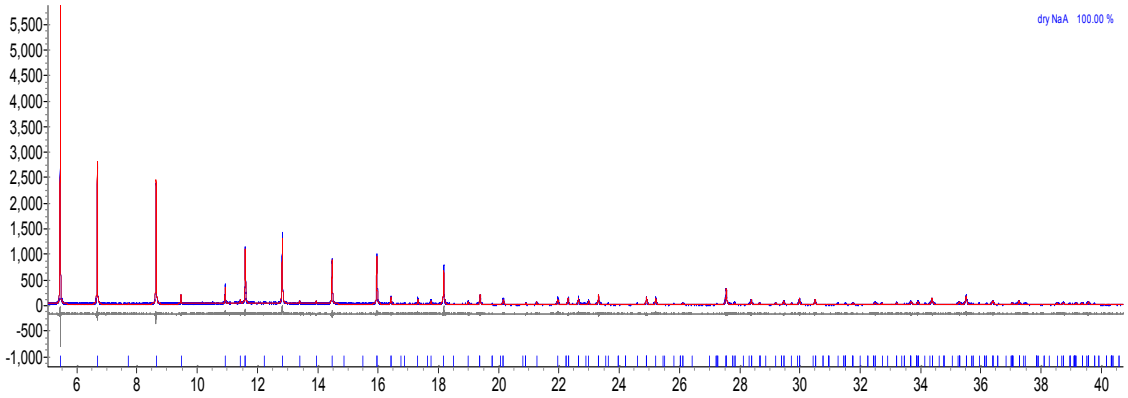

Figure 24 - Rietveld refinement plot of dehydrated Na-A at 300 K.

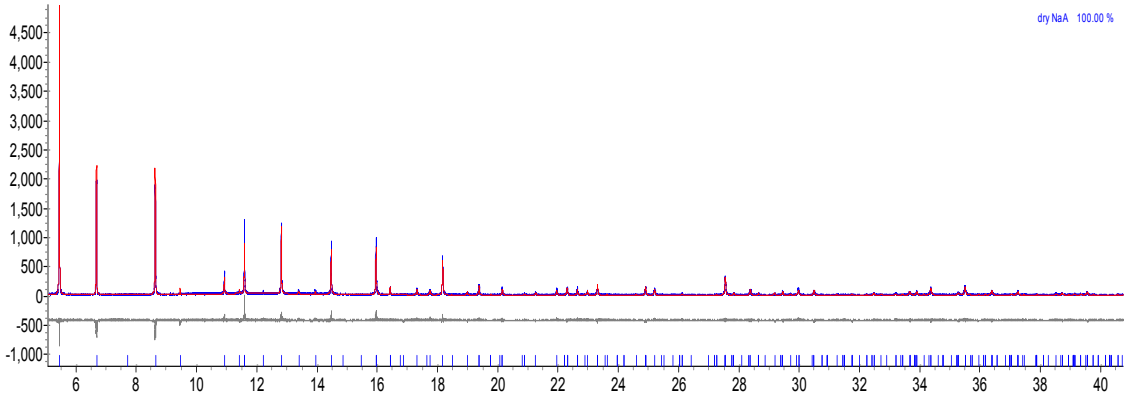

Figure 25 - Rietveld refinement plot of dehydrated Na-A at 200 K.

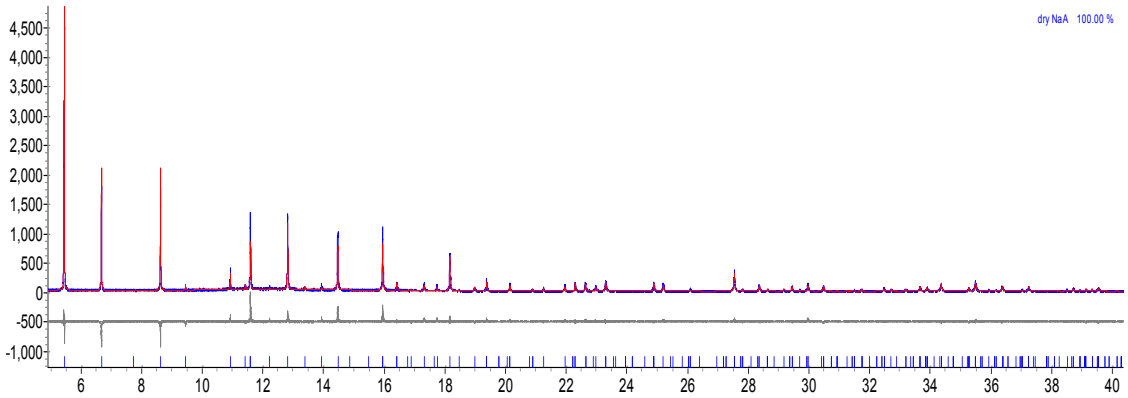

Figure 26 - Rietveld refinement plot of dehydrated Na-A at 100 K.

Dehydrated K-A

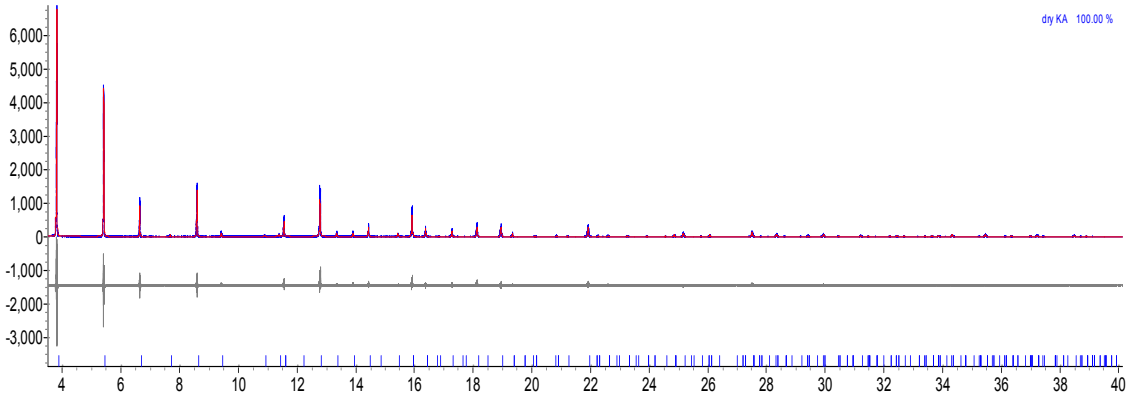

Figure 27 - Rietveld refinement plot of dehydrated K-A at 300 K.

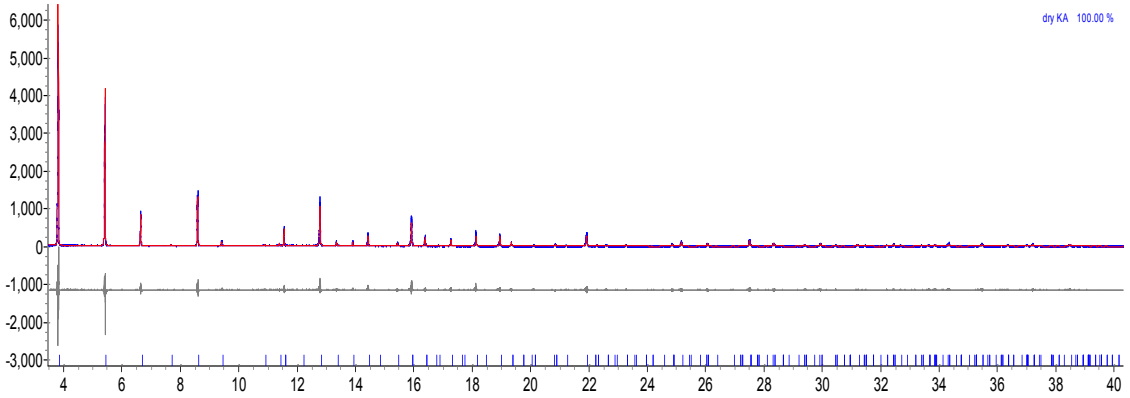

Figure 28 - Rietveld refinement plot of dehydrated K-A at 200 K.

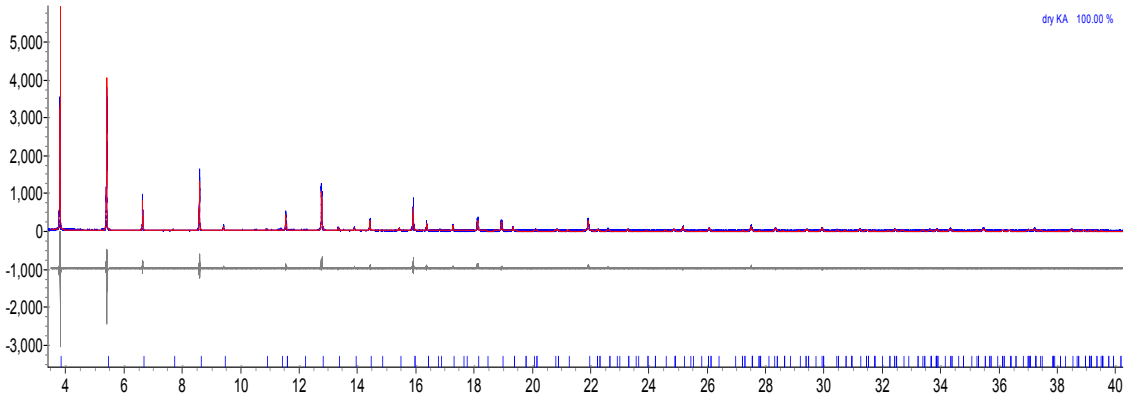

Figure 29 - Rietveld refinement plot of dehydrated K-A at 100 K.

Dehydrated $Rb_{0.79}Na_{0.21}$-A

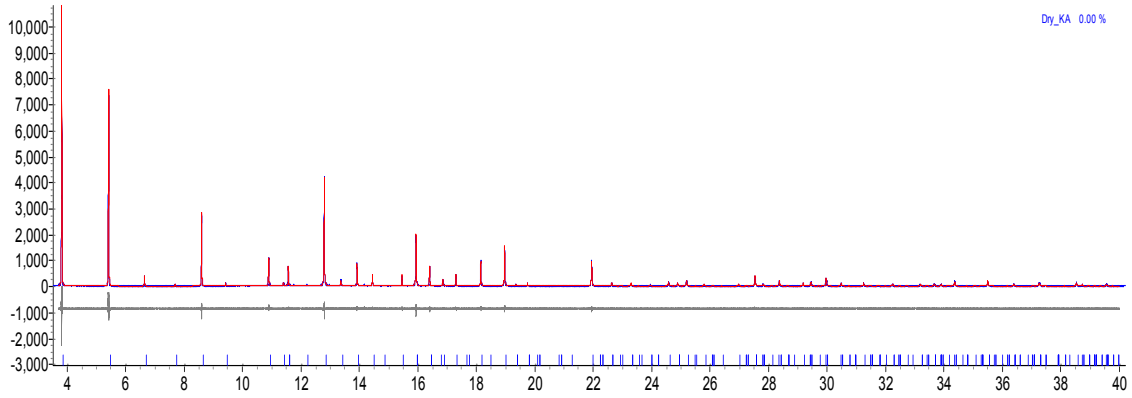

Figure 30 - Rietveld refinement plot of dehydrated $Rb_{0.79}Na_{0.21}$-A at 300 K.

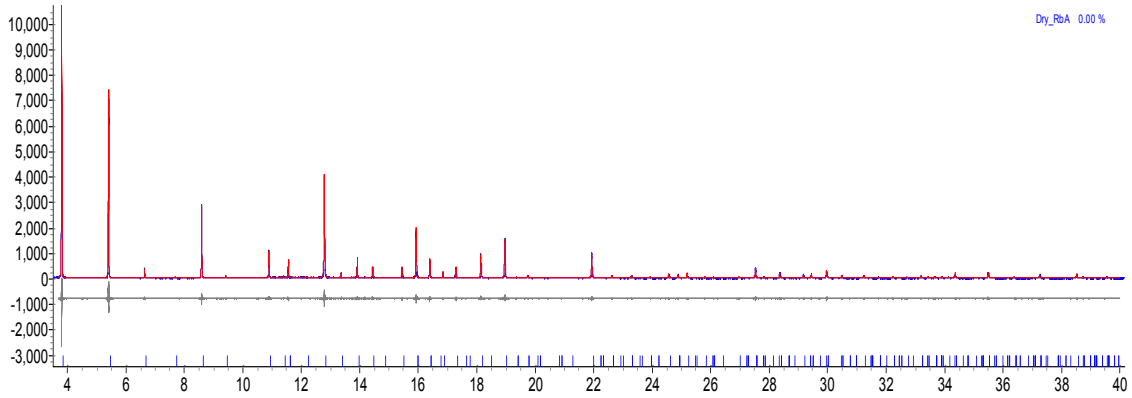

Figure 31 - Rietveld refinement plot of dehydrated $Rb_{0.79}Na_{0.21}$-A at 200 K.

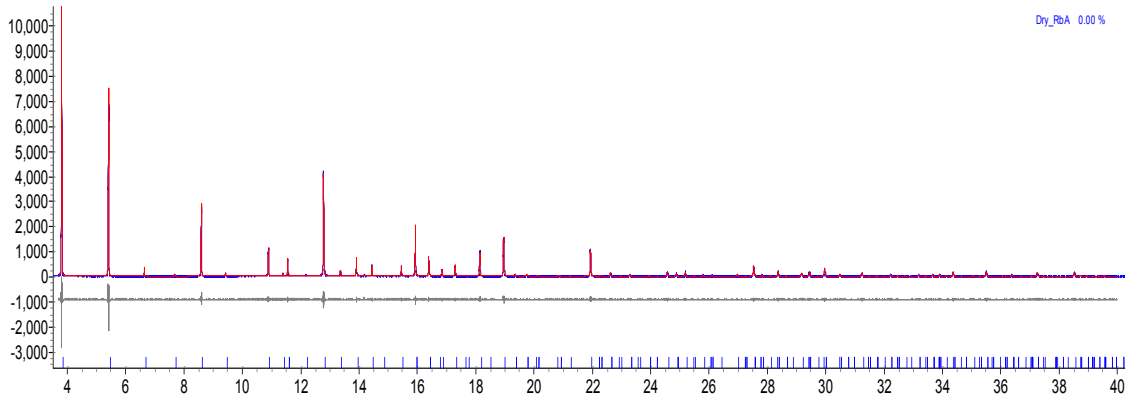

Figure 32 - Rietveld refinement plot of dehydrated $Rb_{0.79}Na_{0.21}$-A at 100 K.

Dehydrated $Cs_{0.58}Na_{0.42}$-A

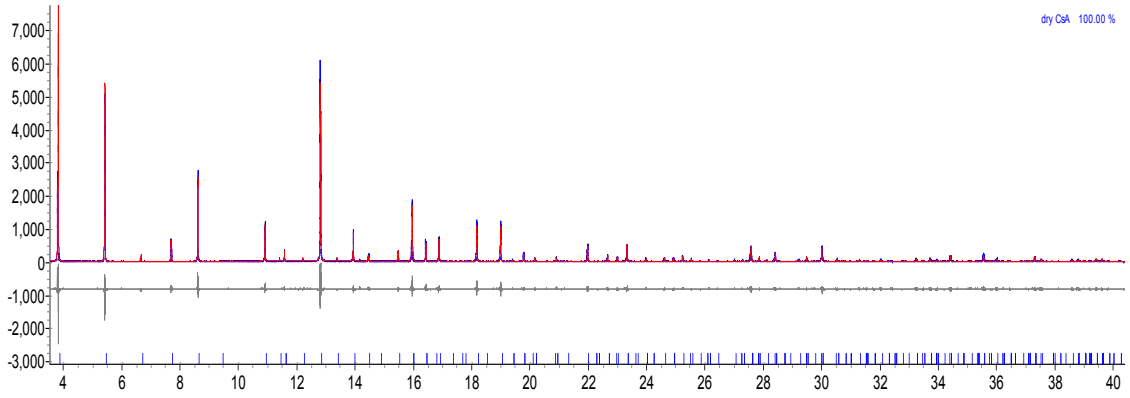

Figure 33 - Rietveld refinement plot of dehydrated $Cs_{0.58}Na_{0.42}$-A at 300 K.

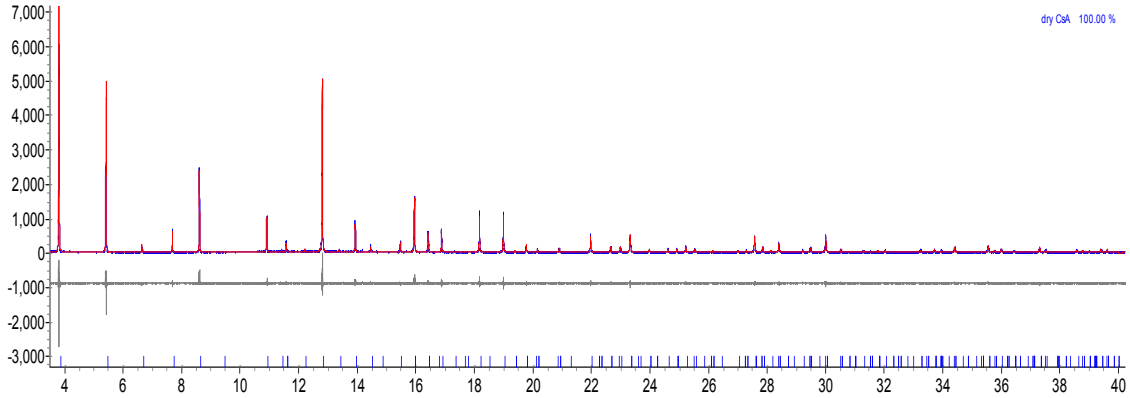

Figure 34 - Rietveld refinement plot of dehydrated $Cs_{0.58}Na_{0.42}$-A at 200 K.

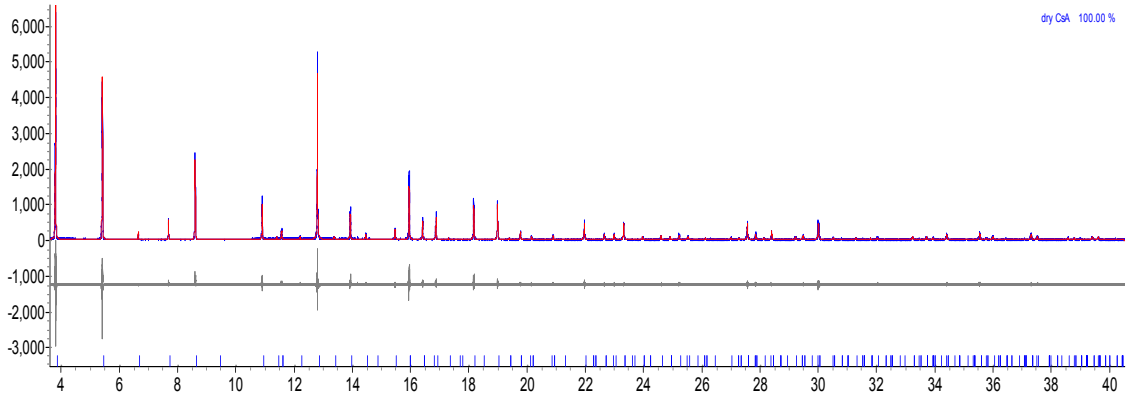

Figure 35 - Rietveld refinement plot of dehydrated $Cs_{0.58}Na_{0.42}$-A at 100 K.