Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Intrusion-extrusion spring performance of –COK-14 zeolite enhanced by structural change

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Supplementary information

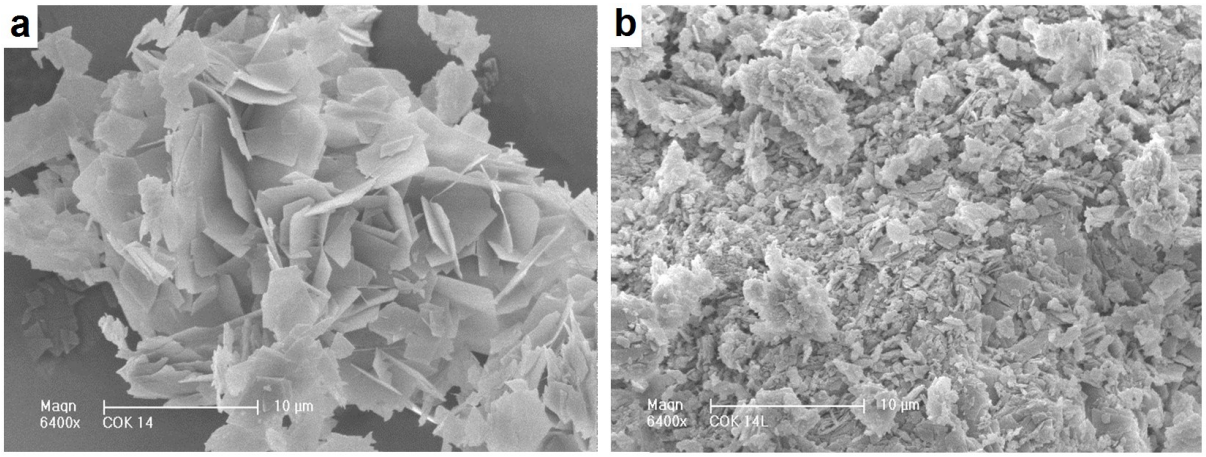

Figure S1. SEM micrographs of the –COK-14 samples before (a) and after intrusion−extrusion experiments with 20M LiCl aqueous solution (b).

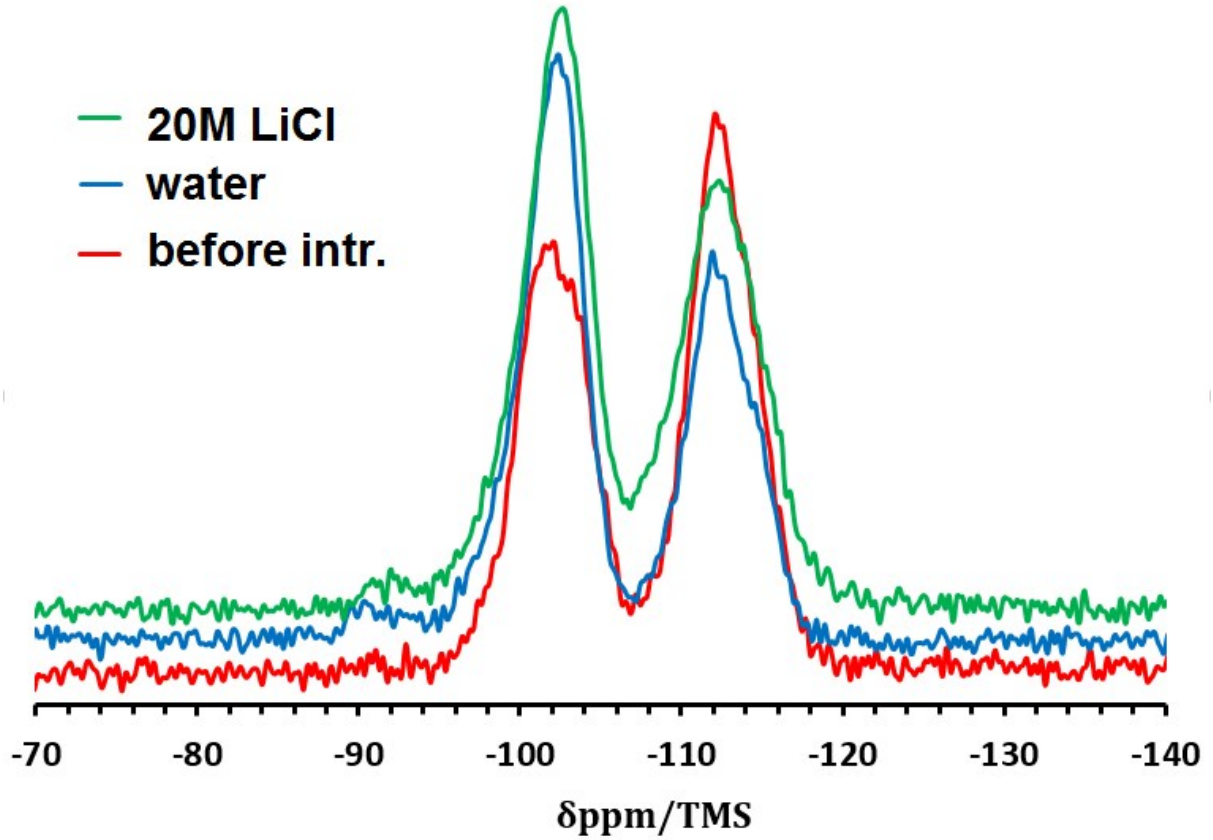

Figure S2. ^{1}H-^{29}Si CP MAS NMR spectra of the –COK-14 samples before and after intrusion−extrusion experiments with water and 20 M LiCl aqueous solutions.

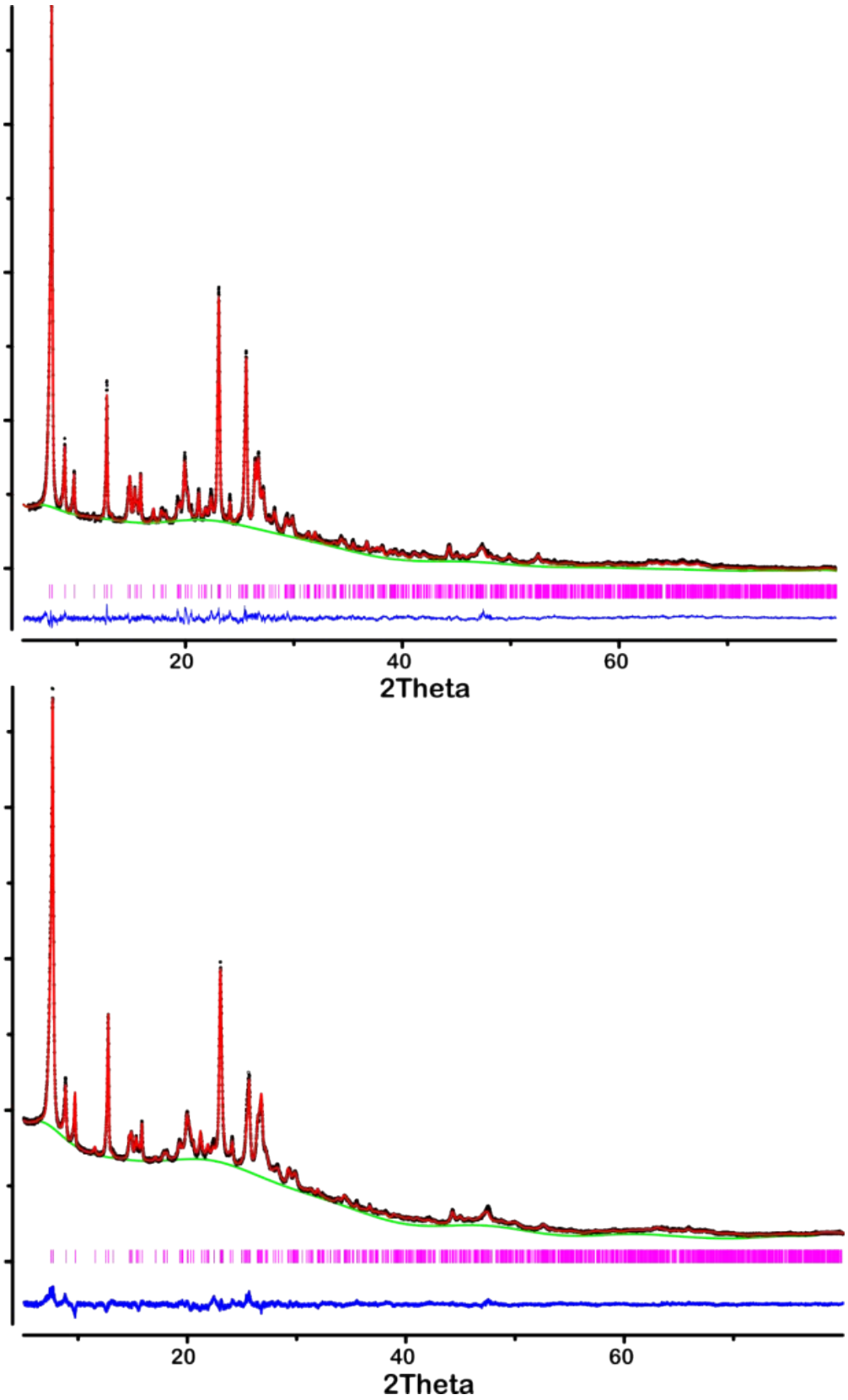

Figure S3. Refined powder patterns of –COK-14, intruded with water (top) and LiCl (bottom). Experimental (black) and calculated (red) XRD patterns as well as the difference profile are shown (blue). The short tick marks below the patterns give the positions of the Bragg reflections.

Water intruded sample, refined structural parameters

Table S1

substructure 1 corresponding to non-intruded –COK-14							substructure 2 with structural break between Sib6 and Sib5						
atom	x	y	z	uiso	occ.	mult.	atom	x	y	z	uiso	occ.	mult.
Si3	0.3154(11)	0.7867(11)	0.2787(19)	0.555(17)	0.031(12)	8	Sib3	0.3093(9)	0.7960(13)	0.2281(17)	0.445(17)	0.043(9)	8
Si4	0.3140(5)	0.7929(10)	0.5139(16)	0.555(17)	0.031(12)	8	Sib4	0.3126(6)	0.7902(11)	0.4940(17)	0.445(17)	0.043(9)	8
Si5	0.3118(10)	0.7930(11)	0.8736(19)	0.555(17)	0.031(12)	8	Sib5	0.3113(13)	0.7922(12)	0.8452(12)	0.445(17)	0.043(9)	8
Si6	0.3626(11)	0.7084(12)	0.0952(19)	0.555(17)	0.031(12)	8	Sib6	0.8890(11)	0.8531(14)	0.1702(22)	0.392(14)	0.043(9)	8
Si7	0.3910(9)	0.7047(11)	0.7525(17)	0.555(17)	0.031(12)	8	Sib7	0.3711(9)	0.7006(12)	0.7042(19)	0.445(17)	0.043(9)	8
Si8	0.2874(16)	0	0.8049(13)	0.555(17)	0.031(12)	4	Sib8	0.2693(16)	0	0.8039(14)	0.445(17)	0.043(9)	4
Si9	0.2301(15)	0.5	0.7907(16)	0.555(17)	0.031(12)	4	Sib9	0.2151(12)	0.5	0.8313(17)	0.445(17)	0.043(9)	4
Si10	0.3341(12)	0.5	0.6830(10)	0.555(17)	0.031(12)	4	Sib10	0.3053(13)	0.5	0.6886(18)	0.445(17)	0.043(9)	4
Si11	0.2294(13)	0.5	0.4693(12)	0.555(17)	0.031(12)	4	Sib11	0.2093(13)	0.5	0.4447(15)	0.445(17)	0.043(9)	4
Si12	0.3022(15)	0.5	0.0593(17)	0.555(17)	0.031(12)	4	Sib12	0.3073(14)	0.5	0.0738(14)	0.445(17)	0.043(9)	4
Si13	0.9870(8)	0.7127(10)	0.1158(15)	0.536(12)	0.031(12)	8	Sib13	1.0106(9)	0.8870(14)	0.1392(10)	0.445(17)	0.043(9)	8
O1	0.3080(16)	0.9030(7)	0.2601(19)	0.555(17)	0.051(8)	8	Ob1	0.3264(11)	0.9072(7)	0.2135(17)	0.445(17)	0.064(12)	8
O2	0.3624(10)	0.7412(16)	0.2237(10)	0.555(17)	0.051(8)	8	Ob2	0.3563(12)	0.7472(14)	0.1771(13)	0.445(17)	0.064(12)	8
O3	0.3395(9)	0.7562(19)	0.4152(16)	0.555(17)	0.051(8)	8	Ob3	0.3155(12)	0.7802(18)	0.3624(17)	0.445(17)	0.064(12)	8
O4	0.2516(14)	0.7359(14)	0.2198(13)	0.555(17)	0.051(8)	8	Ob4	0.2424(10)	0.7744(11)	0.1472(16)	0.445(17)	0.064(12)	8
O5	0.3035(12)	0.9076(6)	0.4992(15)	0.555(17)	0.051(8)	8	Ob5	0.3244(12)	0.9016(7)	0.5413(15)	0.445(17)	0.064(12)	8
O6	0.25	0.75	0.5	0.555(17)	0.051(8)	4	Ob6	0.25	0.75	0.5	0.445(17)	0.064(12)	4
O7	0.3617(7)	0.7730(17)	0.6407(17)	0.555(17)	0.051(8)	8	Ob7	0.3666(7)	0.7209(18)	0.5710(18)	0.445(17)	0.064(12)	8
O8	0.3121(12)	0.7758(19)	0.0048(12)	0.555(17)	0.051(8)	8	Ob81	0.3711(10)	0.7550(19)	-0.0335(16)	0.445(17)	0.064(12)	8
							Ob82	0.8985(17)	0.9048(7)	0.2945(11)	0.392(14)	0.064(12)	8
O9	0.3265(14)	0.9046(7)	0.8564(16)	0.555(17)	0.051(8)	8	Ob9	0.3017(16)	0.9035(7)	0.8714(14)	0.445(17)	0.064(12)	8
O10	0.3627(16)	0.7269(10)	0.8531(12)	0.555(17)	0.051(8)	8	Ob10	0.3233(8)	0.7758(17)	0.7237(10)	0.445(17)	0.064(12)	8
O11	0.3426(16)	0.5959(7)	0.072(4)	0.555(17)	0.051(8)	8	Ob11	0.3437(14)	0.5941(7)	0.0584(21)	0.445(17)	0.064(12)	8
O13	0.3758(12)	0.5944(7)	0.7109(17)	0.555(17)	0.051(8)	8	Ob13	0.3448(14)	0.5955(7)	0.7183(16)	0.445(17)	0.064(12)	8
O14	0.2286(18)	0	0.8398(11)	0.555(17)	0.051(8)	4	Ob14	0.2021(16)	0	0.8001(15)	0.445(17)	0.064(12)	4
O15	0.2747(18)	0	0.6664(12)	0.555(17)	0.051(8)	4	Ob15	0.2760(19)	0	0.6761(17)	0.445(17)	0.064(12)	4
O16	0.2507(11)	0.5	0.9328(15)	0.555(17)	0.051(8)	4	Ob16	0.2446(16)	0.5	0.9708(18)	0.445(17)	0.064(12)	4
O17	0.2889(20)	0.5	0.755(5)	0.555(17)	0.051(8)	4	Ob17	0.2626(11)	0.5	0.765(5)	0.445(17)	0.064(12)	4
O18	0.2980(14)	0.5	0.5452(12)	0.555(17)	0.051(8)	4	Ob18	0.2707(17)	0.5	0.5510(10)	0.445(17)	0.064(12)	4
O19	0.0389(8)	0.7835(14)	0.1925(19)	0.555(17)	0.051(8)	8	Ob19	0.0629(10)	0.8108(10)	0.2058(17)	0.445(17)	0.064(12)	8
O31	0.9840(12)	0.6176(14)	0.1928(11)	0.555(17)	0.051(8)	8	Ob20	0.5184(12)	0.5	0.185(5)	0.445(17)	0.064(12)	4
O21	0.9253(7)	0.7710(18)	0.0814(16)	0.555(17)	0.051(8)	8	Ob21	0.9507(9)	0.8392(17)	0.1504(13)	0.445(17)	0.064(12)	8
O22	0	0.678(4)	0	0.536(12)	0.051(8)	4	Ob22	0	0.887(5)	0	0.445(17)	0.064(12)	4

LiCl intruded sample, refined structural parameters

Table S2

substructure 1 corresponding to non-intruded –COK-14						
atom	x	y	z	uiso	occ.	mult.
Si3	0.3027(8)	0.7851(6)	0.2872(9)	0.373(12)	0.038(21)	8
Si4	0.31442(30)	0.7922(6)	0.5156(9)	0.373(12)	0.038(21)	8
Si5	0.3216(6)	0.7903(7)	0.8609(12)	0.373(12)	0.038(21)	8
Si6	0.3504(7)	0.7087(7)	0.0880(12)	0.373(12)	0.038(21)	8
Si7	0.3975(6)	0.7064(7)	0.7508(10)	0.373(12)	0.038(21)	8
Si8	0.2972(12)	0	0.8033(16)	0.373(12)	0.038(21)	4
Si9	0.2351(11)	0.5	0.7841(15)	0.373(12)	0.038(21)	4
Si10	0.3388(8)	0.5	0.6871(13)	0.373(12)	0.038(21)	4
Si11	0.2275(8)	0.5	0.4736(13)	0.373(12)	0.038(21)	4
Si12	0.2893(10)	0.5	0.0503(16)	0.373(12)	0.038(21)	4
Si13	0.9816(5)	0.7278(20)	0.1163(8)	0.315(10)	0.038(21)	8
O1	0.2994(12)	0.9031(4)	0.2794(15)	0.373(12)	0.057(19)	8
O2	0.3393(15)	0.7448(16)	0.2060(17)	0.373(12)	0.057(19)	8
O3	0.3389(5)	0.7472(10)	0.4181(9)	0.373(12)	0.057(19)	8
O4	0.2364(9)	0.7415(18)	0.2459(19)	0.373(12)	0.057(19)	8
O5	0.3049(8)	0.9071(4)	0.4935(14)	0.373(12)	0.057(19)	8
O6	0.25	0.75	0.5	0.373(12)	0.057(19)	4
O7	0.3599(5)	0.7764(10)	0.6453(9)	0.373(12)	0.057(19)	8
O8	0.3084(8)	0.7748(13)	-0.0176(17)	0.373(12)	0.057(19)	8
O9	0.3366(11)	0.9040(4)	0.8503(19)	0.373(12)	0.057(19)	8
O10	0.3789(10)	0.7270(15)	0.8651(13)	0.373(12)	0.057(19)	8
O11	0.3302(11)	0.5959(4)	0.0648(14)	0.373(12)	0.057(19)	8
O13	0.3803(8)	0.5953(4)	0.7095(12)	0.373(12)	0.057(19)	8
O14	0.2419(14)	0	0.8501(10)	0.373(12)	0.057(19)	4
O15	0.2773(13)	0	0.6624(15)	0.373(12)	0.057(19)	4
O16	0.2404(14)	0.5	0.9210(15)	0.373(12)	0.057(19)	4
O17	0.3003(13)	0.5	0.7736(19)	0.373(12)	0.057(19)	4
O18	0.2962(8)	0.5	0.5529(14)	0.373(12)	0.057(19)	4
O19	0.0329(5)	0.7779(17)	0.2234(14)	0.373(12)	0.057(19)	8
O31	0.9776(16)	0.6125(16)	0.143(4)	0.373(12)	0.057(19)	8
O21	0.9187(5)	0.7786(13)	0.0989(14)	0.373(12)	0.057(19)	8
O22	0	0.740(5)	0	0.315(10)	0.057(19)	4

substructure 2 with structural break between Sib6 and Sib5						
atom	x	y	z	uiso	occ.	mult.
Sib3	0.3087(7)	0.7924(7)	0.2331(11)	0.627(12)	0.078(8)	8
Sib4	0.31286(32)	0.7888(6)	0.4941(10)	0.627(12)	0.078(8)	8
Sib5	0.3169(7)	0.7922(7)	0.8763(16)	0.627(12)	0.078(8)	8
Sib6	0.8775(9)	0.8566(8)	0.1649(16)	0.408(13)	0.078(8)	8
Sib7	0.3816(7)	0.7001(7)	0.7233(13)	0.627(12)	0.078(8)	8
Sib8	0.2719(10)	0	0.8031(17)	0.627(12)	0.078(8)	4
Sib9	0.2167(7)	0.5	0.8252(17)	0.627(12)	0.078(8)	4
Sib10	0.3122(8)	0.5	0.6971(11)	0.627(12)	0.078(8)	4
Sib11	0.2137(8)	0.5	0.4530(15)	0.627(12)	0.078(8)	4
Sib12	0.2973(8)	0.5	0.0664(15)	0.627(12)	0.078(8)	4
Sib13	1.0035(7)	0.8923(9)	0.1362(7)	0.627(12)	0.078(8)	8
Ob1	0.3228(8)	0.9072(4)	0.2333(15)	0.627(12)	0.082(10)	8
Ob2	0.3554(10)	0.7527(7)	0.1744(17)	0.627(12)	0.082(10)	8
Ob3	0.3186(8)	0.7637(14)	0.3672(11)	0.627(12)	0.082(10)	8
Ob4	0.2414(8)	0.7727(13)	0.1534(19)	0.627(12)	0.082(10)	8
Ob5	0.3206(7)	0.9032(4)	0.5284(19)	0.627(12)	0.082(10)	8
Ob6	0.25	0.75	0.5	0.627(12)	0.082(10)	4
Ob7	0.3671(4)	0.7315(12)	0.5890(13)	0.627(12)	0.082(10)	8
Ob81	0.3618(11)	0.7611(10)	0.0129(18)	0.627(12)	0.082(10)	8
Ob82	0.8789(14)	0.9049(4)	0.2870(18)	0.408(13)	0.082(10)	8
Ob9	0.3025(9)	0.9054(4)	0.8781(19)	0.627(12)	0.082(10)	8
Ob10	0.3534(13)	0.7780(10)	0.7887(14)	0.627(12)	0.082(10)	8
Ob11	0.3316(9)	0.5963(4)	0.0490(18)	0.627(12)	0.082(10)	8
Ob13	0.3529(8)	0.5956(4)	0.7289(17)	0.627(12)	0.082(10)	8
Ob14	0.2048(10)	0	0.8020(14)	0.627(12)	0.082(10)	4
Ob15	0.2760(15)	0	0.6726(11)	0.627(12)	0.082(10)	4
Ob16	0.2338(10)	0.5	0.9654(16)	0.627(12)	0.082(10)	4
Ob17	0.2725(12)	0.5	0.7807(33)	0.627(12)	0.082(10)	4
Ob18	0.2756(10)	0.5	0.5598(13)	0.627(12)	0.082(10)	4
Ob19	0.0489(8)	0.8088(8)	0.2081(17)	0.627(12)	0.082(10)	8
Ob20	0.5225(11)	0.5	0.1908(17)	0.627(12)	0.082(10)	4
Ob21	0.9411(8)	0.8611(14)	0.1493(16)	0.627(12)	0.082(10)	8
Ob22	0	0.8904(33)	0	0.627(12)	0.082(10)	4

Bond lengths and distances in refined substructure 2

Table S3

LiCl intruded sample				Water intruded sample			
Vector	Length/Å	Angle	Degrees/°	Vector	Length/Å	Angle	Degrees/°
Sib3_Ob1	1.62982(20)	Ob1_Sib3_Ob2	103.788(8)	Sib3_Ob1	1.62895(19)	Ob1_Sib3_Ob2	102.479(10)
Sib3_Ob2	1.63218(30)	Ob1_Sib3_Ob3	106.050(4)	Sib3_Ob2	1.63126(29)	Ob1_Sib3_Ob3	107.473(4)
Sib3_Ob3	1.63095(20)	Ob1_Sib3_Ob4	109.552(2)	Sib3_Ob3	1.61803(20)	Ob1_Sib3_Ob4	110.508(4)
Sib3_Ob4	1.6326(4)	Ob2_Sib3_Ob3	118.067(11)	Sib3_Ob4	1.6403(4)	Ob2_Sib3_Ob3	119.586(11)
		Ob2_Sib3_Ob4	112.967(16)			Ob2_Sib3_Ob4	112.640(15)
		Ob3_Sib3_Ob4	110.305(15)			Ob3_Sib3_Ob4	109.173(15)
Sib4_Ob3	1.64575(18)	Ob3_Sib4_Ob5	114.181(2)	Sib4_Ob3	1.64473(19)	Ob3_Sib4_Ob5	111.438(3)
Sib4_Ob5	1.63735(20)	Ob3_Sib4_Ob6	110.109(14)	Sib4_Ob5	1.64717(19)	Ob3_Sib4_Ob6	110.897(14)
Sib4_Ob6	1.6498(4)	Ob3_Sib4_Ob7	105.424(13)	Sib4_Ob6	1.6594(4)	Ob3_Sib4_Ob7	102.904(13)
Sib4_Ob7	1.64923(33)	Ob5_Sib4_Ob6	109.578(5)	Sib4_Ob7	1.65799(30)	Ob5_Sib4_Ob6	111.046(6)
		Ob5_Sib4_Ob7	106.785(10)			Ob5_Sib4_Ob7	109.450(12)
		Ob6_Sib4_Ob7	110.634(16)			Ob6_Sib4_Ob7	110.830(15)
Sib5_Ob4	1.62025(32)	Ob4_Sib5_Ob81	107.902(15)	Sib5_Ob4	1.63894(30)	Ob4_Sib5_Ob81	104.065(16)
Sib5_Ob81	1.72617(33)	Ob4_Sib5_Ob9	111.455(12)	Sib5_Ob81	1.7855(4)	Ob4_Sib5_Ob9	110.985(11)
Sib5_Ob9	1.61161(19)	Ob4_Sib5_Ob10	114.720(13)	Sib5_Ob9	1.61516(19)	Ob4_Sib5_Ob10	111.439(12)
Sib5_Ob10	1.61878(26)	Ob81_Sib5_Ob9	107.560(3)	Sib5_Ob10	1.62781(19)	Ob81_Sib5_Ob9	104.253(5)
		Ob81_Sib5_Ob10	107.576(16)			Ob81_Sib5_Ob10	111.957(15)
		Ob9_Sib5_Ob10	107.347(3)			Ob9_Sib5_Ob10	113.525(2)
Sib6_Ob2	1.62699(19)	Ob2_Sib6_Ob82	102.952(7)	Sib6_Ob2	1.62637(19)	Ob2_Sib6_Ob31	104.493(8)
Sib6_Ob82	1.63096(17)	Ob2_Sib6_Ob11	106.760(11)	Sib6_Ob31	1.63104(18)	Ob2_Sib6_Ob11	102.737(14)
Sib6_Ob11	1.62770(30)	Ob2_Sib6_Ob21	113.330(5)	Sib6_Ob11	1.62655(29)	Ob2_Sib6_Ob21	113.982(9)
Sib6_Ob21	1.6267(4)	Ob82_Sib6_Ob11	115.870(11)	Sib6_Ob21	1.6226(4)	Ob31_Sib6_Ob11	115.758(11)
		Ob82_Sib6_Ob21	111.186(14)			Ob31_Sib6_Ob21	109.936(14)
		Ob11_Sib6_Ob21	106.826(16)			Ob11_Sib6_Ob21	109.803(14)
Sib7_Ob7	1.62585(21)	Ob7_Sib7_Ob10	109.603(9)	Sib7_Ob7	1.62505(19)	Ob7_Sib7_Ob10	102.764(11)
Sib7_Ob10	1.62833(18)	Ob7_Sib7_Ob13	109.290(8)	Sib7_Ob10	1.64763(26)	Ob7_Sib7_Ob13	111.409(6)
Sib7_Ob13	1.62188(18)	Ob7_Sib7_Ob19	112.578(15)	Sib7_Ob13	1.63106(18)	Ob7_Sib7_Ob19	114.639(15)
Sib7_Ob19	1.6296(5)	Ob10_Sib7_Ob13	108.301(12)	Sib7_Ob19	1.6377(4)	Ob10_Sib7_Ob13	103.214(14)
		Ob10_Sib7_Ob19	109.466(12)			Ob10_Sib7_Ob19	113.810(11)
		Ob13_Sib7_Ob19	107.494(9)			Ob13_Sib7_Ob19	100.334(9)
Sib8_Ob9	1.63497(19)	Ob9_Sib8_Ob9	106.838(14)	Sib8_Ob9	1.63869(19)	Ob9_Sib8_Ob9	110.099(15)
Sib8_Ob9	1.63497(19)	Ob9_Sib8_Ob14	105.943(10)	Sib8_Ob9	1.63869(19)	Ob9_Sib8_Ob14	109.302(10)
Sib8_Ob14	1.6331(4)	Ob9_Sib8_Ob15	112.707(8)	Sib8_Ob14	1.6343(4)	Ob9_Sib8_Ob15	107.410(8)
Sib8_Ob15	1.63666(19)	Ob9_Sib8_Ob14	105.943(10)	Sib8_Ob15	1.62916(19)	Ob9_Sib8_Ob14	109.302(10)
		Ob9_Sib8_Ob15	112.707(8)			Ob9_Sib8_Ob15	107.410(8)
		Ob14_Sib8_Ob15	112.184(16)			Ob14_Sib8_Ob15	113.274(15)
Sib9_Ob1	1.62639(21)	Ob1_Sib9_Ob1	104.725(16)	Sib9_Ob1	1.62377(21)	Ob1_Sib9_Ob1	105.398(17)
Sib9_Ob1	1.62639(21)	Ob1_Sib9_Ob16	111.899(9)	Sib9_Ob1	1.62377(21)	Ob1_Sib9_Ob16	111.570(10)
Sib9_Ob16	1.63002(23)	Ob1_Sib9_Ob17	106.965(11)	Sib9_Ob16	1.62174(27)	Ob1_Sib9_Ob17	107.684(11)
Sib9_Ob17	1.6261(4)	Ob1_Sib9_Ob16	111.899(9)	Sib9_Ob17	1.62728(32)	Ob1_Sib9_Ob16	111.570(10)
		Ob1_Sib9_Ob17	106.965(11)			Ob1_Sib9_Ob17	107.685(11)
		Ob16_Sib9_Ob17	113.811(16)			Ob16_Sib9_Ob17	112.568(16)
Sib10_Ob13	1.62562(21)	Ob13_Sib10_Ob13	109.407(17)	Sib10_Ob13	1.61406(20)	Ob13_Sib10_Ob13	110.879(17)
Sib10_Ob13	1.62562(21)	Ob13_Sib10_Ob17	107.019(10)	Sib10_Ob13	1.61406(20)	Ob13_Sib10_Ob17	108.939(10)
Sib10_Ob17	1.62722(28)	Ob13_Sib10_Ob18	109.358(10)	Sib10_Ob17	1.62068(30)	Ob13_Sib10_Ob18	107.679(10)
Sib10_Ob18	1.62447(30)	Ob13_Sib10_Ob17	107.019(10)	Sib10_Ob18	1.61832(29)	Ob13_Sib10_Ob17	108.939(10)
		Ob13_Sib10_Ob18	109.358(10)			Ob13_Sib10_Ob18	107.679(10)
		Ob17_Sib10_Ob18	114.560(16)			Ob17_Sib10_Ob18	112.733(16)
Sib11_Ob5	1.63828(19)	Ob5_Sib11_Ob5	110.176(15)	Sib11_Ob5	1.63809(19)	Ob5_Sib11_Ob5	113.459(15)
Sib11_Ob5	1.63827(19)	Ob5_Sib11_Ob15	112.011(8)	Sib11_Ob5	1.63809(19)	Ob5_Sib11_Ob15	111.421(8)
Sib11_Ob15	1.64113(19)	Ob5_Sib11_Ob18	105.475(10)	Sib11_Ob15	1.63675(20)	Ob5_Sib11_Ob18	106.297(10)
Sib11_Ob18	1.6397(4)	Ob5_Sib11_Ob15	112.011(8)	Sib11_Ob18	1.6334(4)	Ob5_Sib11_Ob15	111.421(8)
		Ob5_Sib11_Ob18	105.475(10)			Ob5_Sib11_Ob18	106.297(10)
		Ob15_Sib11_Ob18	111.303(16)			Ob15_Sib11_Ob18	107.496(17)
Sib12_Ob11	1.62809(19)	Ob11_Sib12_Ob11	110.350(15)	Sib12_Ob11	1.63121(19)	Ob11_Sib12_Ob11	106.820(15)
Sib12_Ob11	1.62809(19)	Ob11_Sib12_Ob14	108.389(8)	Sib12_Ob11	1.63121(19)	Ob11_Sib12_Ob14	111.302(8)
Sib12_Ob14	1.63200(19)	Ob11_Sib12_Ob16	107.492(10)	Sib12_Ob14	1.63740(19)	Ob11_Sib12_Ob16	108.768(11)
Sib12_Ob16	1.6327(4)	Ob11_Sib12_Ob14	108.389(8)	Sib12_Ob16	1.6356(4)	Ob11_Sib12_Ob14	111.302(8)
		Ob11_Sib12_Ob16	107.492(10)			Ob11_Sib12_Ob16	108.768(11)
		Ob14_Sib12_Ob16	114.710(16)			Ob14_Sib12_Ob16	109.784(16)
Sib13_Ob19	1.64368(24)	Ob19_Sib13_Ob20	111.960(13)	Sib13_Ob19	1.65668(28)	Ob19_Sib13_Ob20	117.142(11)
Sib13_Ob20	1.64080(18)	Ob19_Sib13_Ob21	104.119(15)	Sib13_Ob20	1.65969(19)	Ob19_Sib13_Ob21	105.381(16)
Sib13_Ob21	1.6414(4)	Ob19_Sib13_Ob22	109.451(11)	Sib13_Ob21	1.6602(4)	Ob19_Sib13_Ob22	110.064(12)
Sib13_Ob22	1.64468(20)	Ob20_Sib13_Ob21	110.265(6)	Sib13_Ob22	1.63936(21)	Ob20_Sib13_Ob21	110.963(7)
		Ob20_Sib13_Ob22	109.995(5)			Ob20_Sib13_Ob22	108.247(3)
		Ob21_Sib13_Ob22	110.929(15)			Ob21_Sib13_Ob22	104.289(15)

Bond lengths and distances in refined substructure 2 , ctnd.

LiCl intruded sample			
Vector	Length/Å	Angle	Degrees/°
		Sib3_Ob1_Sib9	132.800(12)
		Sib3_Ob2_Sib6	129.996(2)
		Sib3_Ob3_Sib4	150.663(5)
		Sib3_Ob4_Sib5	149.573(7)
		Sib4_Ob5_Sib11	144.110(9)
		Sib4_Ob6_Sib4	180.000(0)
		Sib4_Ob7_Sib7	134.365(11)
		Sib5_Ob9_Sib8	146.736(5)
		Sib5_Ob10_Sib7	145.385(5)
		Sib6_Ob11_Sib12	116.758(8)
		Sib7_Ob13_Sib10	163.294(3)
		Sib8_Ob14_Sib12	110.574(16)
		Sib8_Ob15_Sib11	174.997(2)
		Sib9_Ob16_Sib12	130.389(13)
		Sib9_Ob17_Sib10	161.976(5)
		Sib10_Ob18_Sib11	150.869(8)
		Sib7_Ob19_Sib13	137.065(8)
		Sib13_Ob20_Sib13	131.278(10)
		Sib6_Ob21_Sib13	166.876(4)
		Sib13_Ob22_Sib13	180.000(0)

Water intruded sample			
Vector	Length/Å	Angle	Degrees/°
		Sib3_Ob1_Sib9	129.602(13)
		Sib3_Ob2_Sib6	143.238(3)
		Sib3_Ob3_Sib4	165.296(2)
		Sib3_Ob4_Sib5	137.036(10)
		Sib4_Ob5_Sib11	141.999(10)
		Sib4_Ob6_Sib4	180.000(0)
		Sib4_Ob7_Sib7	116.674(12)
		Sib5_Ob9_Sib8	139.818(7)
		Sib5_Ob10_Sib7	125.126(10)
		Sib6_Ob11_Sib12	120.846(8)
		Sib7_Ob13_Sib10	160.706(4)
		Sib8_Ob14_Sib12	115.448(15)
		Sib8_Ob15_Sib11	173.462(2)
		Sib9_Ob16_Sib12	142.333(10)
		Sib9_Ob17_Sib10	175.071(1)
		Sib10_Ob18_Sib11	149.172(9)
		Sib7_Ob19_Sib13	145.683(7)
		Sib13_Ob20_Sib13	142.757(7)
		Sib6_Ob21_Sib13	149.359(8)
		Sib13_Ob22_Sib13	180.000(0)