Revision 1

Supporting Information for

Structuration under Pressure: Spatial Separation of Inserted Water during Pressure-Induced Hydration in Mesolite

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PART I. Supporting Figures

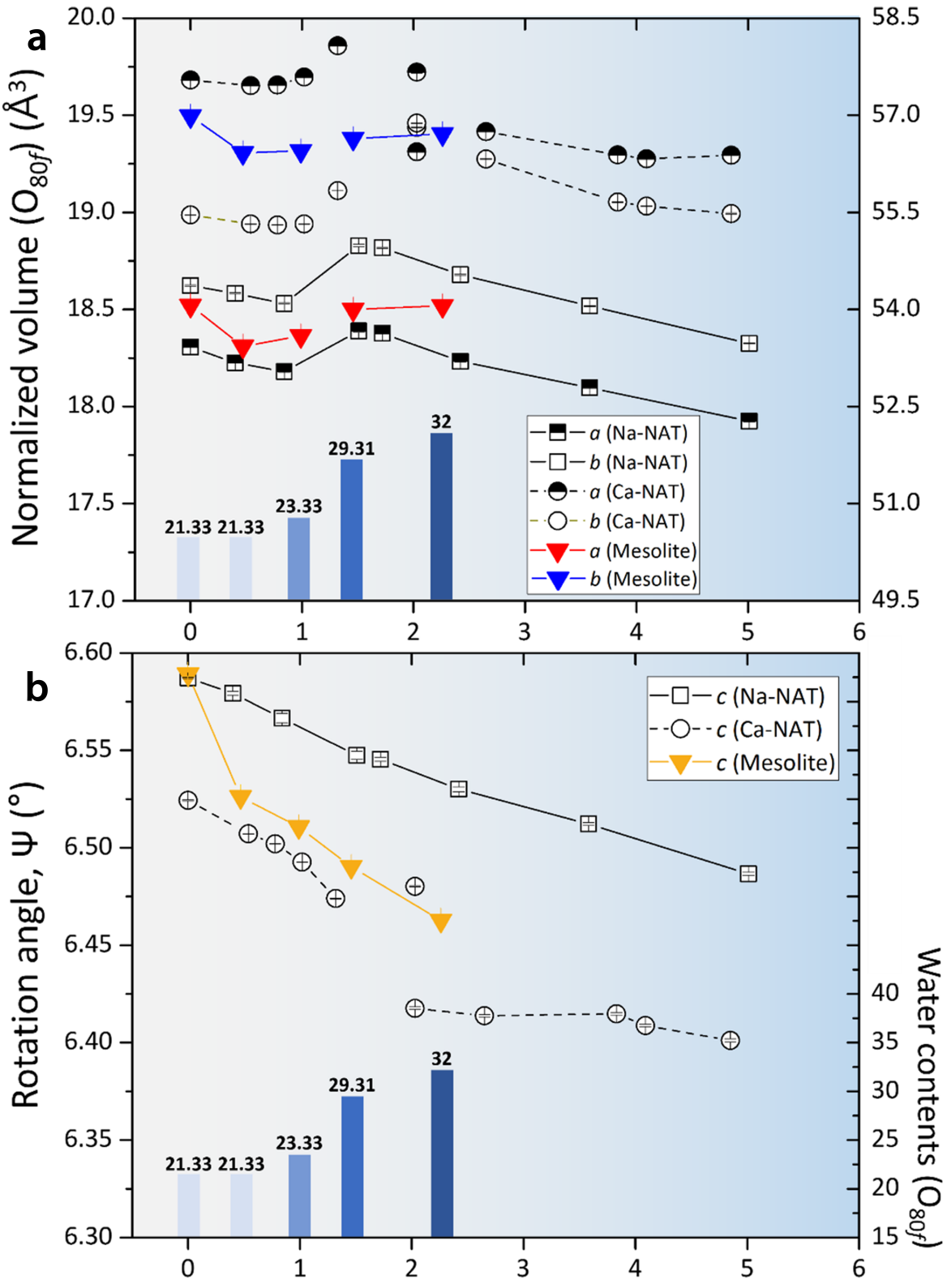

Figure S1. Changes in the lengths of unit cell edges of Na-, Ca-NAT, and mesolite as a function of pressure.

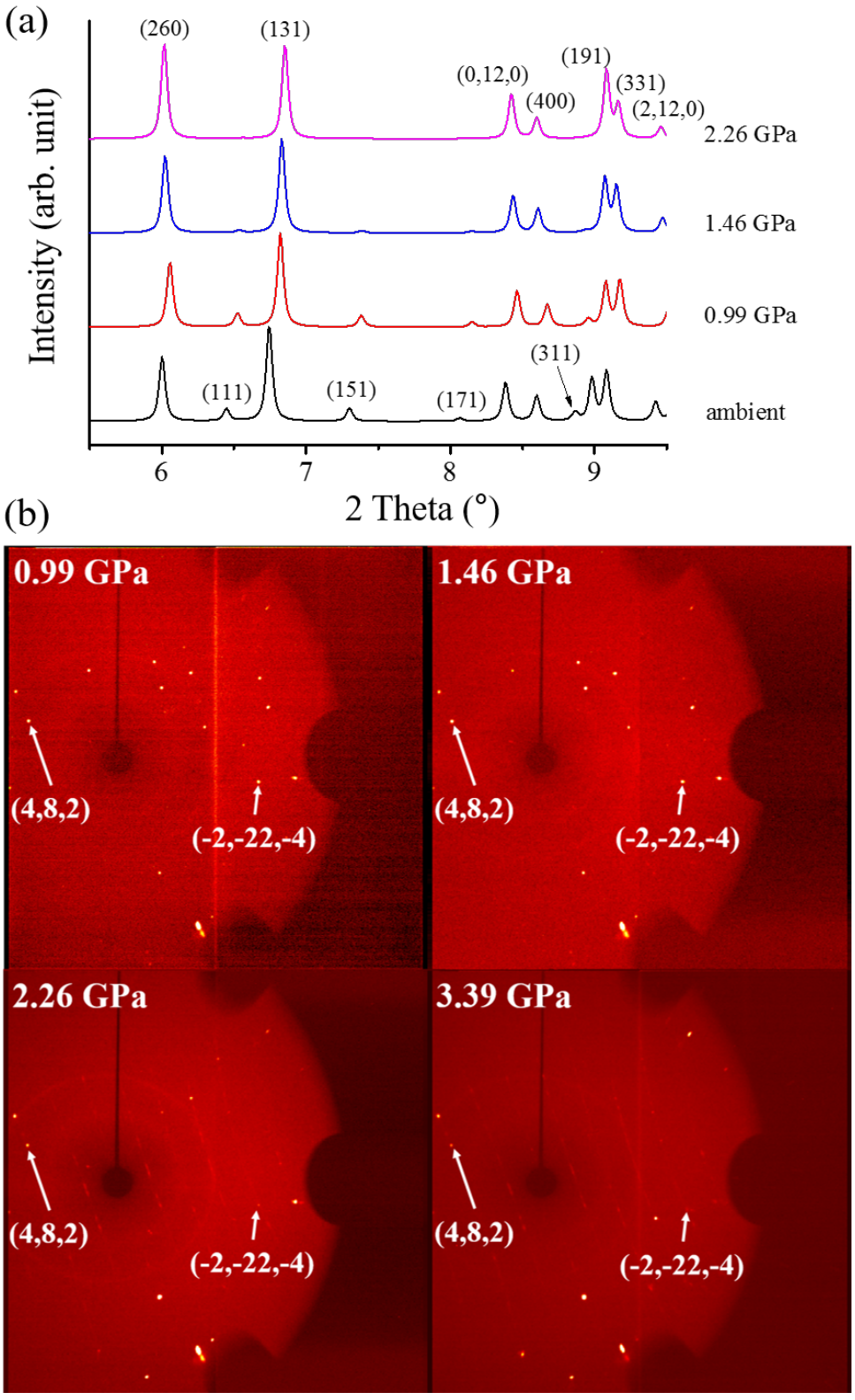

Figure S2. (a) Simulated powder diffraction patterns of mesolite at different pressures, (b) X-ray diffraction spots with Miller indices of $k \neq 3n$.

PART II. Supporting Tables

Table S1. Refined unit cell parameters and volume for mesolite as a function of hydrostatic pressure

Pressure (GPa)	Space group	*a* (Å)	*b* (Å)	*c* (Å)	Volume (Å^3)	H_2O
ambient	*Fdd*2	18.520(2)	56.987(7)	6.5891(9)	6954.0(16)	21.33
0.47	*Fdd*2	18.3101	56.4176	6.5261	6741.57	21.33
0.99	*Fdd*2	18.363(3)	56.451(8)	6.5107(7)	6749.2(17)	23.33
1.46	*Fdd*2	18.500(4)	56.641(11)	6.4903(10)	6801(2)	29.31
2.26	*Fdd*2	18.519(2)	56.713(6)	6.4627(6)	6787.7(13)	32

Table S2a. Final refined atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for mesolite at ambient pressure. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	*y*	*z*	U(eq)
Si(1)	2458(1)	5818(1)	3982(2)	8(1)
Si(2)	1619(1)	5969(1)	7732(2)	8(1)
Si(3)	3480(1)	5698(1)	7713(2)	8(1)
Si(4)	5000	5000	1208(2)	8(1)
Si(5)	4050(1)	4857(1)	4935(1)	7(1)
Al(1)	2983(1)	6124(1)	10141(2)	8(1)
Al(2)	4630(1)	5302(1)	7347(2)	7(1)
Al(3)	2136(1)	5521(1)	139(2)	8(1)
Na(1)	2824(1)	5108(1)	7519(3)	21(1)
Ca(1)	4780(1)	4226(1)	5025(1)	14(1)
O(1)	2656(1)	6032(1)	2484(5)	18(1)
O(2)	3127(1)	5779(1)	5544(4)	15(1)
O(3)	1739(1)	5890(1)	5337(4)	14(1)
O(4)	2268(1)	5581(1)	2724(4)	14(1)
O(5)	1536(1)	5734(1)	9143(4)	14(1)
O(6)	2278(1)	6137(1)	8407(4)	15(1)
O(7)	833(1)	6093(1)	7903(4)	12(1)
O(8)	3605(1)	5920(1)	9217(4)	14(1)
O(9)	2940(1)	5507(1)	8741(4)	15(1)
O(10)	4261(1)	5584(1)	7186(4)	11(1)
O(11)	4303(1)	4931(1)	2631(4)	14(1)
O(12)	5184(1)	4772(1)	-147(4)	15(1)
O(13)	4595(1)	4654(1)	5814(4)	13(1)
O(14)	4066(1)	5086(1)	6357(4)	14(1)
O(15)	3228(1)	4762(1)	4850(4)	11(1)
O(1W)	3036(2)	4816(1)	9980(5)	23(1)
O(2W)	4508(2)	4016(1)	8031(5)	34(1)
O(3W)	5323(2)	4341(1)	1995(6)	40(1)
O(4W)	5683(1)	3931(1)	4854(6)	29(1)
H(1A)	3518(17)	4842(9)	10540(80)	57(16)
H(1B)	2930(30)	4680(8)	9100(90)	80(20)
H(2A)	4110(30)	4041(13)	8930(100)	110(30)
H(2B)	4920(30)	3976(13)	9010(110)	130(30)
H(3A)	5320(30)	4489(6)	1300(90)	64(18)
H(3B)	5460(40)	4212(10)	1000(100)	140(30)
H(4A)	6190(20)	3982(14)	5050(180)	170(40)
H(4B)	5540(30)	3767(5)	5050(110)	90(20)

Table S2b. Anisotropic displacement parameters ($Å^2$x 10^3) for mesolite at ambient pressure. The anisotropic displacement factor exponent takes the form: $-2p^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	8(1)	9(1)	6(1)	0(1)	0(1)	0(1)
Si(2)	7(1)	7(1)	8(1)	0(1)	0(1)	1(1)
Si(3)	7(1)	7(1)	9(1)	0(1)	1(1)	0(1)
Si(4)	10(1)	8(1)	6(1)	0(1)	0(1)	-1(1)
Si(5)	6(1)	7(1)	8(1)	0(1)	0(1)	-1(1)
Al(1)	9(1)	6(1)	8(10	0(1)	1(1)	-1(1)
Al(2)	9(1)	6(1)	7(1)	0(1)	0(1)	0(1)
Al(3)	8(1)	6(1)	9(1)	0(1)	0(1)	-1(1)
Na(1)	20(1)	19(1)	24(1)	-1(1)	1(1)	2(1)
Ca(1)	14(1)	13(1)	16(1)	-1(1)	-1(1)	-1(1)
O(1)	24(1)	14(1)	16(1)	3(1)	4(1)	0(1)
O(2)	15(1)	20(1)	11(1)	0(1)	-4(1)	3(1)
O(3)	10(1)	22(1)	9(1)	-4(1)	0(1)	1(1)
O(4)	20(1)	11(1)	12(1)	-2(1)	-2(1)	-2(1)
O(5)	13(1)	11(1)	17(2)	4(1)	0(1)	2(1)
O(6)	15(1)	14(1)	17(2)	0(1)	-5(1)	-2(1)
O(7)	10(1)	10(1)	17(1)	2(1)	2(1)	1(1)
O(8)	13(1)	14(1)	16(2)	-4(1)	0(1)	1(1)
O(9)	14(1)	13(1)	18(2)	2(1)	6(1)	-4(1)
O(10)	9(1)	7(1)	16(1)	2(1)	2(1)	1(1)
O(11)	13(1)	20(1)	11(1)	4(1)	4(1)	-3(1)
O(12)	22(1)	12(1)	11(1)	-2(1)	3(1)	1(1)
O(13)	12(1)	10(1)	16(1)	1(1)	-4(1)	2(1)
O(14)	15(1)	11(1)	16(1)	-4(1)	1(1)	-2(1)
O(15)	9(1)	10(1)	13(1)	0(1)	0(1)	-1(1)
O(1W)	27(1)	23(1)	18(2)	-2(1)	-3(1)	0(1)
O(2W)	28(2)	51(2)	24(2)	11(2)	12(1)	4(2)
O(3W)	65(2)	26(2)	30(2)	8(2)	23(2)	4(2)
O(4W)	21(1)	19(1)	48(2)	-7(2)	-6(1)	-2(1)

Table S3. Final refined atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Mesolite at 0.99 GPa. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	*y*	*z*	U(eq)
Si(1)	5051(3)	6678(1)	5934(8)	4(1)
Si(2)	5891(3)	6531(1)	2188(8)	6(1)
Si(3)	4027(3)	6800(1)	2195(8)	7(1)
Si(4)	2500	7500	8672(11)	5(2)
Si(5)	3453(3)	7643(1)	4920(8)	8(1)
Al(1)	7032(3)	6126(1)	2289(8)	4(2)
Al(2)	2870(3)	7197(1)	2551(8)	4(2)
Al(3)	5364(4)	6978(1)	9798(9)	8(2)
Na(1)	4717(5)	7403(2)	2411(12)	23(2)
Ca(1)	2709(3)	8275(1)	4895(6)	14(1)
O(1)	4838(8)	6457(2)	7460(20)	16(3)
O(2)	4370(8)	6716(3)	4450(20)	14(4)
O(3)	5781(8)	6611(3)	4632(19)	12(3)
O(4)	5233(8)	6916(2)	7207(19)	13(3)
O(5)	5967(8)	6766(2)	797(19)	11(4)
O(6)	5249(8)	6362(2)	1529(18)	10(4)
O(7)	6672(8)	6410(3)	2022(19)	11(4)
O(8)	3904(8)	6583(3)	685(19)	10(3)
O(9)	4582(8)	6990(3)	1216(19)	11(4)
O(10)	3246(8)	6912(3)	2742(18)	6(3)
O(11)	3207(7)	7577(3)	7295(18)	10(3)
O(12)	2311(7)	7726(2)	10030(20)	12(3)
O(13)	2896(9)	7845(3)	4076(18)	9(3)
O(14)	3424(8)	7411(2)	3497(19)	9(3)
O(15)	4251(8)	7741(3)	5059(19)	12(3)
O(1W)	4415(9)	7689(3)	-80(20)	28(4)
O(2W)	2963(9)	8487(3)	1870(20)	22(4)
O(3W)	1784(8)	8571(3)	5080(20)	21(4)
O(4W)	2134(9)	8155(3)	7910(20)	36(5)
O(5W)	5690(20)	7722(8)	2350(60)	32(18)

Table S4. Final refined atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Mesolite at 1.46 GPa. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	*y*	*z*	U(eq)
Si(1)	5018(5)	6671(2)	25966(17)	6(3)
Si(2)	5905(6)	6532(2)	22215(15)	3(3)
Si(3)	4056(6)	6800(2)	22226(17)	7(3)
Si(4)	2500	7500	28580(20)	1(3)
Si(5)	3434(6)	7648(2)	24803(16)	8(3)
Al(1)	7066(7)	6124(2)	22334(17)	10(3)
Al(2)	2892(6)	7199(2)	22464(15)	4(3)
Al(3)	5394(6)	6968(2)	29860(17)	7(3)
Na(1)	5242(9)	7593(3)	27360(20)	25(5)
Ca(1)	2302(7)	6734(2)	24926(18)	15(4)
Ca(2)	2708(19)	6581(8)	19420(50)	40(13)
O(1)	4786(15)	6455(5)	27440(50)	23(7)
O(2)	4364(18)	6737(6)	24540(50)	38(9)
O(3)	5676(17)	6583(7)	24640(50)	36(9)
O(4)	5293(15)	6887(5)	27310(40)	23(8)
O(5)	5970(20)	6758(6)	20840(50)	43(10)
O(6)	5315(15)	6357(5)	21490(40)	15(7)
O(7)	6647(15)	6405(5)	22280(40)	10(7)
O(8)	3960(16)	6571(5)	20760(40)	21(8)
O(9)	4604(14)	6991(5)	21270(30)	5(7)
O(11)	3187(15)	7595(5)	27250(40)	19(8)
O(10)	3270(14)	6916(5)	22610(30)	9(7)
O(12)	2286(13)	7713(4)	29940(40)	4(6)
O(13)	2884(15)	7837(5)	23990(40)	11(7)
O(14)	3438(14)	7403(5)	23420(40)	9(6)
O(15)	4231(17)	7749(7)	25000(40)	29(9)
O(1W)	4344(19)	7709(6)	-150(50)	43(10)
O(2W)	2980(20)	8506(7)	2190(60)	62(11)
O(3W)	3190(20)	6443(8)	25230(70)	70(14)
O(4W)	2040(30)	8157(9)	7690(70)	96(16)
O(5W)	4350(20)	7283(8)	27380(60)	60(12)
O(6W)	1870(50)	6880(20)	19960(140)	90(50)

Table S5. Final refined atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Mesolite at 2.26 GPa. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	*y*	*z*	U(eq)
Si(1)	5001(4)	6670(1)	25990(30)	18(6)
Si(2)	5894(7)	6526(3)	22192(18)	13(5)
Si(3)	4061(7)	6809(2)	22194(18)	14(5)
Si(4)	2500	7500	28560(30)	21(7)
Si(5)	3432(7)	7642(2)	24753(17)	11(5)
Al(1)	7053(8)	6128(3)	22410(20)	14(6)
Al(2)	2909(8)	7201(3)	22480(20)	16(6)
Al(3)	5405(8)	6971(2)	29920(20)	13(6)
Na(1)	5275(11)	7587(4)	27340(30)	35(7)
Ca(1)	2248(11)	6735(4)	24770(30)	42(7)
Ca(2)	2755(13)	6597(5)	19540(40)	24(9)
O(1)	4726(18)	6464(5)	27400(50)	23(9)
O(2)	4372(17)	6726(6)	24690(60)	30(10)
O(3)	5640(20)	6599(7)	24730(70)	64(13)
O(4)	5289(18)	6884(6)	27300(50)	27(9)
O(5)	5890(20)	6747(6)	20610(60)	39(12)
O(6)	5349(16)	6353(6)	21360(40)	17(10)
O(7)	6680(20)	6409(7)	22300(50)	33(12)
O(8)	4030(20)	6586(6)	20650(50)	38(12)
O(9)	4588(15)	6979(5)	21230(40)	9(9)
O(11)	3162(16)	7573(5)	27320(50)	18(10)
O(10)	3272(19)	6915(7)	22430(50)	23(11)
O(12)	2218(17)	7718(5)	29910(50)	17(8)
O(13)	2870(17)	7823(6)	23940(40)	22(10)
O(14)	3418(18)	7412(5)	23280(50)	17(10)
O(15)	4220(20)	7754(7)	24960(50)	24(11)
O(1W)	4315(19)	7693(6)	-300(60)	65(11)
O(2W)	3010(30)	8507(8)	2150(80)	108(16)
O(3W)	3170(20)	6435(8)	25270(60)	55(15)
O(4W)	1940(30)	8158(11)	7240(100)	170(20)
O(5W)	4360(20)	7275(8)	27640(60)	56(15)
O(6W)	1790(30)	6888(10)	20320(80)	100(20)

Table S6. Selected interatomic distances (Å) and angles (°) for mesolite as a function of pressures.

	ambient	0.99 GPa	1.46 GPa	2.26 GPa
Na(1)-O(1W)	2.351(3)	2.340(18)	2.41(4)	2.42(4)
Na(1)-O(1W)	2.357(3)	2.356(18)	2.49(4)	2.45(4)
Na(1)-O(5W)		2.54(5)	2.41(5)	2.46(5)
Na(1)-O(9)	2.422(3)	2.468(17)	2.48(3)	2.57(4)
Na(1)-O(14)	2.426(3)	2.477(17)	2.54(3)	2.49(4)
Na(1)-O(15)	2.588(3)	2.568(17)	2.58(4)	2.66(4)
Na(1)-O(15)	2.748(3)	2.710(17)	2.76(4)	2.73(5)
Ca(1)-O(2W)	2.369(3)	2.355(14)	2.30(4)	2.23(5)
Ca(1)-O(3W)	2.329(3)	2.385(16)	2.34(5)	2.43(5)
Ca(1)-O(4W)	2.374(3)	2.330(16)	2.26(5)	2.28(6)
Ca(1)-O(6W)				3.12(6)
Ca(1)-O(5)	2.515(2)	2.513(15)	2.53(4)	2.57(4)
Ca(1)-O(7)	2.561(2)	2.523(15)	2.70(3)	2.68(5)
Ca(1)-O(10)	2.520(2)	2.480(15)	2.56(3)	2.63(4)
Ca(1)-O(13)	2.515(2)	2.509(15)	2.53(3)	2.58(4)
Ca(2)-O(2W)			2.26(6)	2.28(5)
Ca(2)-O(3W)			2.97(5)	3.00(5)
Ca(2)-O(4W)			1.92(6)	2.11(6)
Ca(2)-O(6W)			2.31(11)	2.49(7)
Ca(2)-O(6)			2.50(5)	2.60(4)
Ca(2)-O(7)			2.60(5)	2.69(5)
Ca(2)-O(8)			2.47(5)	2.47(5)
Ca(2)-O(10)			2.99(5)	2.77(5)
Si(1)-O(1)-Al(1)	148.45(18)	146.6(10)	145(2)	146(2)
Si(1)-O(4)-Al(3)	133.39(16)	134.0(9)	139.9(19)	140(2)
Si(1)-O(3)-Si(2)	133.59(15)	131.3(9)	141(2)	142(3)
Si(1)-O(2)-Si(3)	153.57(17)	150.4(10)	149(2)	146(3)
Si(2)-O(6)-Al(1)	136.47(17)	135.9(9)	134.6(19)	136(2)
Si(2)-O(7)-Al(1)	136.84(15)	136.7(11)	144(2)	138(3)
Si(2)-O(5)-Al(3)	135.33(15)	135.6(9)	137(2)	142(3)
Si(3)-O(8)-Al(1)	129.65(15)	129.2(9)	131(2)	138(3)
Si(3)-O(10)-Al(2)	134.66(15)	134.0(11)	136(2)	135(3)
Si(3)-O(9)-Al(3)	135.42(16)	135.9(10)	133.4(18)	138(2)
Si(4)-O(11)-Si(5)	144.27(17)	142.1(10)	140.3(18)	141(2)
Si(4)-O(12)-Al(2)	139.67(17)	140.3(9)	143.9(16)	140(2)
Si(5)-O(13)-Al(2)	126.83(15)	127.4(9)	129.7(19)	134(3)
Si(5)-O(14)-Al(2)	143.45(16)	144.2(10)	141.9(18)	143(3)
Si(5)-O(15)-Al(3)	131.62(14)	133.7(12)	134(3)	137(3)