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New data on the crystal chemistry of the natural 2D zeolites latiumite and tuscanite

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Table S1. Atom coordinates, equivalent and anisotropic displacement parameters (in Å^2) and site occupancy factors (s.o.f.) for latiumute.

Site	x	y	z	U_{eq}	s.o.f.	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca1	0.88319(5)	0.25629(14)	0.18942(5)	0.0128(2)	$Ca_{0.845(8)}Na_{0.095(8)}Sr_{0.06}$	0.0114(3)	0.0122(3)	0.0151(3)	-0.0010(3)	0.0044(2)	-0.0002(3)
Ca2	0.20735(5)	0.25348(16)	0.14632(6)	0.0151(2)	$Ca_{0.858(8)}Na_{0.142(8)}$	0.0128(3)	0.0170(4)	0.0161(4)	-0.0023(3)	0.0051(2)	0.0015(3)
Ca3	0.11637(5)	0.73936(13)	0.45442(5)	0.0106(2)	$Ca_{0.990(8)}Na_{0.010(8)}$	0.0092(3)	0.0096(3)	0.0126(3)	-0.0003(3)	0.0026(2)	-0.0023(3)
S	0.03784(6)	0.78031(17)	0.13977(7)	0.0101(2)	$S_{0.897(4)}$	0.0080(4)	0.0103(4)	0.0121(4)	0.0018(3)	0.0031(3)	0.0010(3)
Si1	0.37785(6)	0.74005(17)	0.07191(6)	0.00635(15)	$Si_{1.00}$	0.0065(3)	0.0063(3)	0.0065(3)	0.0000(3)	0.0024(2)	0.0001(3)
Si2	0.34317(6)	0.25169(18)	0.47810(6)	0.00787(16)	$Si_{1.00}$	0.0077(3)	0.0076(3)	0.0085(3)	0.0002(4)	0.0026(2)	-0.0007(3)
Si3	0.82453(7)	0.70703(15)	0.35529(7)	0.00749(18)	$Si_{1.00}$	0.0080(3)	0.0073(4)	0.0069(3)	0.0000(3)	0.0017(3)	-0.0008(3)
Al1	0.38395(6)	0.7512(2)	0.35208(7)	0.00635(16)	$Al_{1.00}$	0.0063(3)	0.0060(4)	0.0066(3)	-0.0002(4)	0.0017(3)	-0.0001(4)
Al2	0.65164(6)	0.73990(19)	0.08298(7)	0.00665(17)	$Al_{1.00}$	0.0065(3)	0.0059(4)	0.0074(4)	0.0002(4)	0.0018(3)	-0.0002(4)
A	0.57420(11)	0.2526(3)	0.27401(12)	0.0175(5)	$O_{0.719(6)}K_{0.281(6)}$	0.0236(8)	0.0128(7)	0.0180(7)	0.0013(7)	0.0092(5)	-0.0023(7)
O1	0.68992(18)	0.0615(4)	0.05198(19)	0.0116(4)	$O_{1.00}$	0.0136(10)	0.0084(10)	0.0109(10)	0.0020(8)	0.0008(8)	-0.0013(8)
O2	0.51542(17)	0.7197(5)	0.1011(2)	0.0161(5)	$O_{1.00}$	0.0082(9)	0.0221(12)	0.0188(10)	0.0024(10)	0.0053(8)	0.0025(9)
O3	0.33617(18)	0.0455(4)	0.04667(19)	0.0105(4)	$O_{1.00}$	0.0145(10)	0.0079(9)	0.0103(9)	0.0013(8)	0.0057(8)	0.0023(8)
O4	0.34053(18)	0.6273(4)	0.19484(19)	0.0109(4)	$O_{1.00}$	0.0129(10)	0.0110(10)	0.0090(9)	0.0017(8)	0.0033(8)	-0.0002(8)
O5	0.33846(19)	0.0791(4)	0.3480(2)	0.0135(4)	$O_{1.00}$	0.0149(10)	0.0114(11)	0.0142(10)	0.0012(8)	0.0043(8)	0.0032(8)
O6	0.53195(18)	0.7235(6)	0.4144(2)	0.0183(5)	$O_{1.00}$	0.0128(10)	0.0241(12)	0.0162(10)	-0.0022(11)	0.0014(8)	0.0019(10)
O7	0.30773(18)	0.5594(4)	0.4360(2)	0.0128(4)	$O_{1.00}$	0.0133(10)	0.0105(10)	0.0160(10)	0.0026(8)	0.0063(8)	0.0015(8)
O8	0.24122(18)	0.1241(4)	0.5351(2)	0.0122(4)	$O_{1.00}$	0.0130(10)	0.0137(10)	0.0113(10)	-0.0033(9)	0.0059(8)	-0.0033(9)
O9	0.94012(18)	0.5317(4)	0.3956(2)	0.0119(4)	$O_{1.00}$	0.0070(9)	0.0132(10)	0.0151(10)	-0.0005(9)	0.0026(8)	-0.0012(8)
O10	0.8388(2)	0.0168(5)	0.3519(2)	0.0188(5)	$O_{1.00}$	0.0345(14)	0.0082(11)	0.0145(11)	-0.0013(9)	0.0083(10)	-0.0060(10)

O11	0.74747(18)	0.5928(4)	0.2169(2)	0.0117(4)	$O_{1.00}$	0.0119(10)	0.0116(11)	0.0085(9)	-0.0006(8)	-0.0018(8)	0.0007(8)
O12	0.9117(2)	0.8138(6)	0.0802(2)	0.0250(6)	$O_{1.00}$	0.0128(11)	0.0350(16)	0.0253(12)	-0.0045(11)	0.0026(9)	0.0041(10)
O13	0.1048(2)	0.8275(5)	0.0478(2)	0.0178(6)	$O_{0.897(4)}$	0.0150(12)	0.0221(14)	0.0194(12)	0.0062(11)	0.0101(10)	0.0005(10)
O14	0.0642(2)	0.5178(5)	0.1995(2)	0.0187(5)	$O_{1.00}$	0.0206(12)	0.0137(11)	0.0257(13)	0.0027(10)	0.0130(10)	0.0021(9)
O15	0.0728(2)	0.9810(5)	0.2448(2)	0.0199(5)	$O_{1.00}$	0.0249(13)	0.0143(11)	0.0189(12)	-0.0005(10)	0.0041(10)	0.0003(10)

Table S2. Atom coordinates, equivalent and anisotropic displacement parameters (in Å^2) and site occupancy factors (s.o.f.) for tuscanite.

Site	x	y	z	U_{eq}	s.o.f.	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca1	0.19148(2)	0.72350(9)	0.18896(5)	0.01243(19)	$Ca_{0.876(6)}Na_{0.079(6)}Sr_{0.045}$	0.0111(3)	0.0126(3)	0.0138(3)	0.00077(19)	0.0039(2)	0.0001(2)
Ca2	0.35399(3)	0.72594(11)	0.14587(6)	0.0152(2)	$Ca_{0.835(6)}Na_{0.165(6)}$	0.0130(4)	0.0171(4)	0.0158(3)	0.0023(2)	0.0048(3)	-0.0012(2)
Ca3	0.30801(2)	0.24049(9)	0.45473(5)	0.01060(19)	$Ca_{0.981(6)}Na_{0.019(6)}$	0.0093(3)	0.0098(3)	0.0124(3)	-0.00007(19)	0.0025(2)	0.0018(2)
S	0.26906(3)	0.19933(13)	0.14020(7)	0.0113(2)	$S_{0.929(2)}$	0.0094(4)	0.0114(4)	0.0131(4)	-0.0012(3)	0.0033(3)	-0.0005(3)
Si1	0.43865(3)	0.24003(12)	0.07234(6)	0.00713(16)	Si1.00	0.0072(4)	0.0071(3)	0.0072(3)	0.0002(2)	0.0023(3)	-0.0001(3)
Si2	0.42174(3)	0.72543(12)	0.47864(7)	0.00832(16)	Si1.00	0.0085(4)	0.0082(3)	0.0085(3)	0.0000(3)	0.0028(3)	0.0003(3)
Si3	0.16167(3)	0.27279(12)	0.35433(6)	0.00853(16)	Si1.00	0.0096(4)	0.0082(3)	0.0077(3)	0.0007(2)	0.0025(3)	0.0007(3)
Al1	0.44175(3)	0.22911(13)	0.35250(7)	0.00703(16)	Al1.00	0.0074(4)	0.0067(4)	0.0072(3)	-0.0001(3)	0.0025(3)	0.0002(3)
Al2	0.07546(3)	0.23563(13)	0.08261(7)	0.00699(17)	Al1.00	0.0075(4)	0.0063(4)	0.0072(3)	-0.0003(3)	0.0022(3)	0.0001(3)
A	0.03728(6)	0.7449(2)	0.27281(12)	0.0175(5)	$O_{0.773(4)}K_{0.227(4)}$	0.0233(9)	0.0123(7)	0.0182(8)	-0.0013(5)	0.0080(6)	-0.0012(5)
O1	0.09658(8)	0.9164(3)	0.05158(16)	0.0110(4)	$O_{1.00}$	0.0103(10)	0.0098(9)	0.0112(9)	-0.0017(7)	0.0005(8)	0.0016(7)
O2	0.00732(8)	0.2301(3)	0.10119(18)	0.0167(4)	$O_{1.00}$	0.0089(10)	0.0249(11)	0.0168(10)	-0.0021(8)	0.0045(9)	-0.0003(8)
O3	0.41981(8)	0.9334(3)	0.04746(16)	0.0108(4)	$O_{1.00}$	0.0153(10)	0.0080(8)	0.0106(8)	-0.0012(7)	0.0062(8)	-0.0020(7)
O4	0.41956(8)	0.3486(3)	0.19498(16)	0.0116(4)	$O_{1.00}$	0.0114(10)	0.0132(9)	0.0105(9)	-0.0009(7)	0.0038(8)	0.0015(8)
O5	0.41978(8)	0.8994(3)	0.35014(16)	0.0131(4)	$O_{1.00}$	0.0156(10)	0.0122(9)	0.0122(9)	0.0000(7)	0.0052(8)	-0.0022(8)

O6	0.01583(9)	0.2414(3)	0.41420(18)	0.0184(4)	$O_{1.00}$	0.0116(10)	0.0247(11)	0.0168(10)	0.0021(8)	0.0007(9)	0.0012(8)
O7	0.40299(8)	0.4211(3)	0.43522(16)	0.0129(4)	$O_{1.00}$	0.0127(10)	0.0120(9)	0.0158(9)	-0.0022(7)	0.0069(9)	-0.0017(7)
O8	0.37117(8)	0.8548(3)	0.53575(16)	0.0131(4)	$O_{1.00}$	0.0152(10)	0.0130(9)	0.0140(9)	0.0023(7)	0.0091(8)	0.0040(8)
O9	0.21970(8)	0.4473(3)	0.39544(16)	0.0119(4)	$O_{1.00}$	0.0084(9)	0.0128(9)	0.0134(9)	-0.0008(7)	0.0017(8)	-0.0002(7)
O10	0.16926(9)	-0.0354(3)	0.35147(16)	0.0200(5)	$O_{1.00}$	0.0376(14)	0.0094(9)	0.0137(9)	0.0010(7)	0.0085(10)	0.0045(9)
O11	0.12283(8)	0.3866(3)	0.21609(16)	0.0123(4)	$O_{1.00}$	0.0138(10)	0.0113(9)	0.0104(8)	-0.0001(7)	0.0014(8)	-0.0005(8)
O12	0.20596(9)	0.1676(4)	0.08147(19)	0.0187(5)	$O_{0.929(2)}$	0.0067(11)	0.0277(12)	0.0210(11)	0.0040(9)	0.0029(10)	-0.0026(9)
O13	0.30230(9)	0.1514(4)	0.04798(19)	0.0244(5)	$O_{1.00}$	0.0214(12)	0.0316(11)	0.0238(11)	-0.0080(9)	0.0123(10)	-0.0028(10)
O14	0.28248(9)	0.4623(3)	0.19931(17)	0.0179(4)	$O_{1.00}$	0.0193(11)	0.0121(9)	0.0259(10)	-0.0031(8)	0.0121(10)	-0.0021(8)
O15	0.28678(9)	-0.0001(3)	0.24569(17)	0.0189(4)	$O_{1.00}$	0.0225(12)	0.0140(9)	0.0188(10)	0.0024(8)	0.0039(10)	0.0020(8)