Table 4.

Anisotropic thermal parameters with standard deviations in parentheses, for lawsonite at 110 K.

atom	U11	U22	U33	U12	U13	U23
Ca	0.00358 (6)	0.0048 (1)	0.00342 (6)	-0.00026 (9)	-0.0012 (1)	-0.00001 (6)
Al	0.0020 (2)	0.0027 (2)	0.0025 (1)	-0.0004 (1)	0.00020 (9)	-0.00033 (8)
Ala	0.0023 (2)	0.0021 (2)	0.0018 (1)	0.0002 (1)	0.00042 (9)	0.00000 (8)
Si	0.0027 (1)	0.0024 (2)	0.00242 (9)	-0.0002 (2)	0.0000 (2)	-0.00004 (8)
Sia	0.0025 (1)	0.0030 (2)	0.00224 (9)	0.0005 (2)	0.0003 (2)	-0.00011 (8)
O1	0.0066 (3)	0.0044 (4)	0.0023 (2)	0.0014 (3)	-0.0009 (5)	0.0000 (2)
O2	0.0039 (1)	0.0053 (2)	0.0048 (1)	-0.0016 (4)	0.0005 (3)	-0.0028 (4)
O2a	0.0039 (1)	0.0053 (2)	0.0048 (1)	0.0014 (4)	0.0015 (3)	-0.0025 (3)
O2b	0.0039 (1)	0.0053 (2)	0.0048 (1)	-0.0024 (4)	0.0011 (3)	-0.0030 (3)
O2c	0.0039 (1)	0.0053 (2)	0.0048 (1)	-0.0021 (4)	-0.0018 (3)	0.0011 (4)
O3	0.0031 (3)	0.0039 (4)	0.0040 (2)	0.0001 (4)	0.0007 (4)	0.0013 (2)
O3a	0.0044 (3)	0.0039 (4)	0.0037 (2)	0.0002 (4)	-0.0004 (4)	-0.0009 (2)
O4	0.0044 (3)	0.0027 (4)	0.0045 (2)	0.0021 (4)	0.0028 (4)	0.0001 (2)
O4a	0.0053 (4)	0.0045 (4)	0.0046 (2)	0.0000 (5)	-0.0018 (4)	-0.0012 (2)
O5	0.0128 (4)	0.0072 (4)	0.0051 (2)	-0.0003 (4)	-0.0030 (5)	0.0006 (3)

Anisotropic thermal parameters with standard deviations in parentheses, for lawsonite at 155 K.

atom	U11	U22	U33	U12	U13	U23
Ca	0.00513 (6)	0.0063 (1)	0.00415 (6)	0	0	0.00002 (7)
Al	0.0025 (2)	0.0026 (2)	0.0025 (1)	-0.0002 (1)	-0.00008 (7)	-0.00028 (9)
Ala	0.0027 (2)	0.0032 (2)	0.0027 (1)	-0.0004 (1)	-0.00025 (7)	0.00019 (9)
Si	0.0029 (1)	0.0034 (2)	0.00255 (9)	0	0	0.00006 (8)
Sia	0.0034 (1)	0.0033 (2)	0.00248 (9)	0	0	-0.00004 (8)
O1	0.0083 (2)	0.0053 (3)	0.0022 (2)	0	0	-0.0002 (3)
O2	0.0056 (2)	0.0062 (3)	0.0052 (2)	-0.0019 (2)	0.0013 (1)	-0.0014 (2)
O2a	0.0034 (2)	0.0051 (3)	0.0044 (2)	-0.0009 (2)	-0.0003 (1)	0.0009 (2)
O3	0.0041 (3)	0.0046 (4)	0.0041 (2)	0	0	0.0009 (2)
O3a	0.0040 (3)	0.0044 (4)	0.0041 (2)	0	0	-0.0013 (2)
O4	0.0049 (3)	0.0036 (4)	0.0047 (2)	0	0	0.0000 (2)
O4a	0.0059 (3)	0.0049 (5)	0.0057 (2)	0	0	-0.0016 (2)
O5	0.0199 (3)	0.0086 (4)	0.0055 (2)	0	0	0.0008 (3)

Anisotropic thermal parameters with standard deviations in parentheses, for lawsonite at 233 K.

atom	U11	U22	U33	U12	U13	U23
Ca	0.00667 (7)	0.0085 (1)	0.00584 (7)	0	0	-0.0001 (1)
Al	0.0033 (3)	0.0036 (2)	0.0033 (1)	-0.0002 (2)	-0.0003 (1)	-0.0004 (1)
Ala	0.0029 (3)	0.0038 (2)	0.0040 (1)	-0.0004 (2)	-0.0003 (1)	0.0002 (1)
Si	0.0035 (2)	0.0039 (2)	0.0033 (1)	0	0	0.0000 (1)
Sia	0.0042 (2)	0.0039 (2)	0.0033 (1)	0	0	-0.0002 (1)
O1	0.0103 (2)	0.0059 (4)	0.0033 (2)	0	0	0.0006 (4)
O2	0.0059 (4)	0.0074 (4)	0.0066 (2)	-0.0024 (3)	0.0014 (2)	-0.0022 (2)
O2a	0.0047 (4)	0.0066 (4)	0.0057 (2)	-0.0014 (3)	-0.0005 (2)	0.0013 (2)
O3	0.0051 (6)	0.0046 (6)	0.0051 (3)	0	0	0.0012 (3)
O3a	0.0047 (5)	0.0056 (6)	0.0056 (3)	0	0	-0.0016 (3)
O4	0.0052 (5)	0.0050 (6)	0.0067 (3)	0	0	0.0007 (3)
O4a	0.0065 (5)	0.0060 (7)	0.0092 (3)	0	0	-0.0026 (3)
O5	0.0266 (4)	0.0111 (5)	0.0075 (3)	0	0	0.0003 (5)

Anisotropic thermal parameters with standard deviations in parentheses, for lawsonite at 295 K.

atom	U11	U22	U33	U12	U13	U23
Ca	0.00843 (9)	0.0108 (2)	0.00713 (8)	0	0	0
Al	0.00409 (9)	0.0045 (1)	0.00440 (9)	-0.00029 (6)	0.00010 (6)	-0.00030 (6)
Si	0.00487 (8)	0.0045 (1)	0.00388 (8)	0	0	0
O1	0.0131 (3)	0.0077 (4)	0.0037 (3)	0	0	0
O2	0.0066 (1)	0.0082 (2)	0.0073 (1)	-0.0023 (1)	0.0013 (1)	-0.0021 (1)
O3	0.0060 (2)	0.0056 (3)	0.0062 (2)	0	0	0.0014 (2)
O4	0.0071 (2)	0.0060 (3)	0.0114 (2)	0	0	0.0026 (2)
O5	0.0364 (6)	0.0142 (6)	0.0086 (3)	0	0	0

Anisotropic thermal parameters with standard deviations in parentheses, for lawsonite at 410 K.

atom	U11	U22	U33	U12	U13	U23
Ca	0.00981 (8)	0.0136 (2)	0.00948 (9)	0	0	0
Al	0.00461 (9)	0.0058 (1)	0.00568 (9)	-0.00029 (6)	0.00008 (6)	-0.00043 (6)
Si	0.00534 (8)	0.0053 (1)	0.00487 (8)	0	0	0
O1	0.0151 (3)	0.0095 (4)	0.0044 (3)	0	0	0
O2	0.0073 (1)	0.0097 (2)	0.0090 (1)	-0.0026 (1)	0.0014 (1)	-0.0025 (1)
O3	0.0070 (2)	0.0065 (3)	0.0078 (2)	0	0	0.0022 (2)
O4	0.0079 (2)	0.0071 (3)	0.0127 (2)	0	0	0.0027 (2)
O5	0.0436 (7)	0.0177 (6)	0.0113 (4)	0	0	0

Anisotropic thermal parameters with standard deviations in parentheses, for lawsonite at 500 K.

atom	U11	U22	U33	U12	U13	U23
Ca	0.0141 (1)	0.0185 (2)	0.0121 (1)	0	0	0
Al	0.0067 (1)	0.0077 (2)	0.0072 (1)	-0.00026 (7)	0.00000 (7)	-0.00065 (7)
Si	0.00753 (9)	0.0065 (2)	0.00590 (9)	0	0	0
O1	0.0199 (4)	0.0122 (5)	0.0057 (3)	0	0	0
O2	0.0097 (2)	0.0119 (2)	0.0112 (2)	-0.0031 (1)	0.0016 (1)	-0.0031 (1)
O3	0.0096 (2)	0.0085 (3)	0.0100 (2)	0	0	0.0027 (2)
O4	0.0107 (2)	0.0091 (3)	0.0145 (2)	0	0	0.0030 (2)
O5	0.0556 (9)	0.0244 (8)	0.0140 (4)	0	0	0