

Table 4 Anisotropic thermal parameters for Johnsburg serendibite

	U11	U22	U33	U12	U13	U23
T1	.0097(5)	.0081(5)	.0061(5)	.0066(4)	.0023(4)	.0028(4)
T2	.0069(2)	.0070(2)	.0062(2)	.0042(2)	.0018(2)	.0029(2)
T3	.0063(3)	.0055(3)	.0055(3)	.0037(2)	.0021(2)	.0027(2)
T4	.0058(9)	.0065(9)	.0076(9)	.0027(8)	.0020(7)	.0038(7)
T5	.0077(3)	.0075(2)	.0079(2)	.0048(2)	.0027(2)	.0019(2)
T6	.0065(2)	.0060(2)	.0056(2)	.0040(2)	.0022(2)	.0022(2)
M1	.0063(4)	.0058(4)	.0050(4)	.0041(3)	.0018(3)	.0021(3)
M2	.0059(4)	.0054(4)	.0054(4)	.0035(3)	.0021(3)	.0019(3)
M3	.0063(3)	.0081(3)	.0063(3)	.0048(2)	.0025(2)	.0032(2)
M4	.0079(3)	.0088(3)	.0083(3)	.0055(2)	.0033(2)	.0041(2)
M5	.0042(3)	.0061(3)	.0055(3)	.0037(3)	.0028(2)	.0042(2)
M6	.0044(3)	.0066(3)	.0076(3)	.0037(3)	.0027(2)	.0044(2)
M7	.0066(3)	.0056(3)	.0060(3)	.0040(2)	.0025(2)	.0025(2)
M8	.0100(2)	.0097(2)	.0085(2)	.0067(2)	.0040(2)	.0045(2)
M9	.0062(2)	.0105(2)	.0107(2)	.0040(2)	.0029(2)	.0052(2)
O1	.0099(7)	.0106(7)	.0109(7)	.0070(6)	.0027(6)	.0039(6)
O2	.0105(7)	.0100(7)	.0074(6)	.0071(6)	.0028(5)	.0035(5)
O3	.0130(7)	.0116(7)	.0129(7)	.0071(6)	.0045(6)	.0017(6)
O4	.0080(7)	.0077(6)	.0070(6)	.0044(6)	.0033(5)	.0029(5)
O5	.0094(7)	.0094(7)	.0092(7)	.0056(6)	.0013(6)	.0026(5)
O6	.0072(7)	.0091(7)	.0105(7)	.0048(6)	.0024(5)	.0040(6)
O7	.0128(7)	.0106(7)	.0131(7)	.0064(6)	.0077(6)	.0063(6)
O8	.0080(7)	.0081(6)	.0091(6)	.0049(6)	.0023(5)	.0041(5)
O9	.0154(8)	.0101(7)	.0089(7)	.0093(6)	.0033(6)	.0040(6)
O10	.0097(7)	.0097(7)	.0100(7)	.0050(6)	.0015(6)	.0044(6)
O11	.0087(7)	.0098(7)	.0123(7)	.0058(6)	.0040(6)	.0046(6)
O12	.0085(7)	.0082(6)	.0085(6)	.0051(6)	.0001(5)	.0015(5)
O13	.0127(7)	.0097(7)	.0108(7)	.0074(6)	.0052(6)	.0038(6)

O14	.0094(7)	.0081(6)	.0076(6)	.0054(6)	.0034(5)	.0035(5)
O15	.0085(7)	.0107(7)	.0089(6)	.0069(6)	.0031(5)	.0037(6)
O16	.0089(7)	.0100(7)	.0075(6)	.0050(6)	.0023(5)	.0009(5)
O17	.0103(7)	.0084(6)	.0088(6)	.0058(6)	.0043(6)	.0051(5)
O18	.0110(7)	.0106(7)	.0088(6)	.0067(6)	.0029(6)	.0043(5)
O19	.0101(7)	.0100(7)	.0118(7)	.0053(6)	.0067(6)	.0039(6)
O20	.0198(8)	.0184(8)	.0099(7)	.0148(7)	.0064(6)	.0052(6)

Note: The standard deviations of the last digit are in parentheses.

The temperature factor expression is:

$$T = \exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)]$$

Anisotropic thermal parameters for serendibite (5151)

Table 4

	U11	U22	U33	U12	U13	U23
T1	.0074(6)	.0068(5)	.0055(5)	.0049(5)	.0020(4)	.0023(4)
T2	.0068(3)	.0071(3)	.0064(3)	.0041(3)	.0018(2)	.0030(2)
T3	.0053(3)	.0051(3)	.0054(3)	.0031(3)	.0015(3)	.0025(2)
T4	.006(1)	.006(1)	.007(1)	.0028(9)	.0025(9)	.0036(9)
T5	.0074(3)	.0076(3)	.0089(3)	.0043(3)	.0029(2)	.0017(2)
T6	.0061(3)	.0058(3)	.0052(3)	.0035(2)	.0022(2)	.0018(2)
M1	.0043(4)	.0037(4)	.0042(4)	.0023(4)	.0014(3)	.0020(3)
M2	.0052(4)	.0051(4)	.0047(4)	.0030(4)	.0020(3)	.0020(3)
M3	.0055(3)	.0083(3)	.0066(3)	.0045(3)	.0029(2)	.0037(2)
M4	.0035(3)	.0047(3)	.0042(3)	.0027(3)	.0020(2)	.0023(2)
M5	.0053(3)	.0079(3)	.0074(3)	.0045(3)	.0035(2)	.0050(2)
M6	.0038(3)	.0067(3)	.0072(3)	.0031(3)	.0027(3)	.0046(3)
M7	.0036(3)	.0034(3)	.0036(3)	.0021(3)	.0013(2)	.0016(2)
M8	.0117(2)	.0111(2)	.0094(2)	.0082(2)	.0049(2)	.0057(2)
M9	.0065(2)	.0119(2)	.0116(2)	.0039(2)	.0032(2)	.0064(2)
O1	.0109(9)	.0130(8)	.0104(8)	.0088(8)	.0035(7)	.0044(7)
O2	.0109(8)	.0107(8)	.0080(8)	.0076(7)	.0036(7)	.0036(6)
O3	.0125(9)	.0107(8)	.0127(8)	.0054(8)	.0047(7)	.0006(7)
O4	.0074(8)	.0082(8)	.0081(7)	.0040(7)	.0036(6)	.0034(6)
O5	.0092(8)	.0083(8)	.0087(8)	.0049(7)	.0006(7)	.0023(6)
O6	.0063(8)	.0069(8)	.0109(8)	.0035(7)	.0017(6)	.0036(6)
O7	.0109(9)	.0097(8)	.0133(8)	.0049(7)	.0067(7)	.0049(7)
O8	.0075(8)	.0068(7)	.0103(8)	.0039(7)	.0017(6)	.0034(6)
O9	.0124(9)	.0095(8)	.0074(8)	.0074(7)	.0024(7)	.0029(6)
O10	.0081(8)	.0095(8)	.0074(8)	.0041(7)	.0010(6)	.0038(6)
O11	.0079(8)	.0105(8)	.0114(8)	.0054(7)	.0039(7)	.0040(7)
O12	.0081(8)	.0068(8)	.0076(7)	.0041(7)	-.0006(6)	.0004(6)
O13	.0128(9)	.0098(8)	.0112(8)	.0075(7)	.0052(7)	.0038(7)

O14	.0092(8)	.0092(8)	.0074(7)	.0056(7)	.0027(6)	.0038(6)
O15	.0082(8)	.0095(8)	.0070(7)	.0054(7)	.0022(6)	.0022(6)
O16	.0072(8)	.0097(8)	.0082(8)	.0037(7)	.0023(6)	.0016(6)
O17	.0079(8)	.0074(7)	.0086(8)	.0044(7)	.0028(6)	.0042(6)
O18	.0107(9)	.0103(8)	.0086(8)	.0062(7)	.0013(7)	.0039(7)
O19	.0103(8)	.0085(8)	.0094(8)	.0052(7)	.0061(7)	.0027(6)
O20	.0179(9)	.0168(9)	.0089(8)	.0143(8)	.0053(7)	.0048(7)

Anisotropic thermal parameters for serendibite (5152)

Table 4

	U11	U22	U33	U12	U13	U23
T1	0.0090(6)	0.0064(5)	0.0059(6)	0.0044(5)	0.0013(4)	0.0023(5)
T2	0.0092(4)	0.0084(4)	0.0075(4)	0.0045(3)	0.0012(3)	0.0030(3)
T3	0.0069(4)	0.0061(4)	0.0062(4)	0.0033(3)	0.0008(3)	0.0024(3)
T4	0.007(1)	0.005(1)	0.008(1)	0.002(1)	0.002(1)	0.003(1)
T5	0.0096(4)	0.0082(4)	0.0101(4)	0.0039(3)	0.0027(3)	0.0021(3)
T6	0.0087(4)	0.0067(4)	0.0067(4)	0.0040(3)	0.0019(3)	0.0020(3)
M1	0.0055(5)	0.0060(5)	0.0058(5)	0.0030(4)	0.0007(4)	0.0026(4)
M2	0.0069(5)	0.0061(5)	0.0058(5)	0.0031(4)	0.0019(4)	0.0024(4)
M3	0.0069(3)	0.0092(3)	0.0076(3)	0.0045(3)	0.0024(3)	0.0040(3)
M4	0.0080(3)	0.0081(3)	0.0084(3)	0.0046(3)	0.0026(3)	0.0038(3)
M5	0.0071(3)	0.0092(3)	0.0087(3)	0.0046(3)	0.0028(3)	0.0050(3)
M6	0.0066(4)	0.0083(4)	0.0088(4)	0.0037(3)	0.0020(3)	0.0047(3)
M7	0.0062(4)	0.0056(3)	0.0058(3)	0.0034(3)	0.0014(3)	0.0022(3)
M8	0.0150(3)	0.0125(3)	0.0107(3)	0.0088(3)	0.0046(2)	0.0062(2)
M9	0.0089(3)	0.0127(3)	0.0132(3)	0.0031(2)	0.0027(2)	0.0066(2)
O1	0.0118(9)	0.014(1)	0.013(1)	0.0079(8)	0.0033(8)	0.0044(8)
O2	0.0143(9)	0.0106(9)	0.0083(9)	0.0080(8)	0.0028(8)	0.0021(8)
O3	0.0148(9)	0.012(1)	0.014(1)	0.0054(8)	0.0055(8)	0.0010(8)
O4	0.0105(9)	0.0083(9)	0.0085(9)	0.0041(8)	0.0023(8)	0.0027(8)
O5	0.0119(9)	0.0069(9)	0.0096(9)	0.0039(8)	-0.0003(8)	0.0019(8)
O6	0.0087(9)	0.0087(9)	0.0125(9)	0.0034(8)	0.0009(8)	0.0036(8)
O7	0.0128(9)	0.012(1)	0.015(1)	0.0034(8)	0.0068(8)	0.0055(8)
O8	0.0080(9)	0.0084(9)	0.0130(9)	0.0035(8)	0.0017(8)	0.0047(8)
O9	0.0148(8)	0.012(1)	0.0083(9)	0.0079(8)	0.0033(8)	0.0035(8)
O10	0.0134(9)	0.0130(9)	0.0079(8)	0.0052(8)	0.0001(8)	0.0046(8)
O11	0.0113(9)	0.0117(9)	0.0115(9)	0.0060(8)	0.0040(8)	0.0040(8)
O12	0.0113(9)	0.008(1)	0.0095(9)	0.0049(8)	-0.0002(8)	0.0000(8)
O13	0.0164(9)	0.0110(9)	0.0104(9)	0.0077(8)	0.0046(8)	0.0025(8)

O14	0.0104(9)	0.0108(9)	0.0087(9)	0.0053(8)	0.0024(8)	0.0048(8)
O15	0.0114(9)	0.0122(9)	0.0069(9)	0.0073(8)	0.0022(8)	0.0023(8)
O16	0.0114(9)	0.0096(9)	0.0096(9)	0.0040(8)	0.0027(8)	0.0022(8)
O17	0.010(1)	0.0085(8)	0.0096(9)	0.0038(8)	0.0028(8)	0.0052(8)
O18	0.0104(9)	0.0116(9)	0.0103(9)	0.0045(8)	0.0002(8)	0.0036(8)
O19	0.0143(9)	0.0093(9)	0.012(1)	0.0048(8)	0.0078(8)	0.0046(8)
O20	0.0224(9)	0.017(1)	0.0097(9)	0.0147(8)	0.0062(8)	0.0054(8)
