

[noprocess]

Table 5. Crystallographic coordinates and equivalent isotropic (\AA^2) and anisotropic temperature factors ($\text{\AA}^2 \cdot 10^4$) of biotite .

Atom	x/a	y/b	z/c	B _{eq}	b ₁₁ [*]	b ₂₂ [*]	b ₃₃ [*]	b ₁₂ [*]	b ₁₃ [*]	b ₂₃ [*]
A4 (1M polytype)										
O1	0.0130(7)	0	0.1704(4)	1.69(8)	190(10)	32(4)	41(4)	0	3(6)	0
O2	0.3272(5)	0.2284(3)	0.1692(3)	1.73(6)	136(8)	54(3)	44(2)	-16(4)	22(4)	-2(2)
O3	0.1316(4)	0.1690(3)	0.3916(2)	1.17(5)	100(7)	35(2)	29(2)	-2(4)	10(3)	0(2)
O4	0.1280(6)	0.5	0.3972(4)	1.34(8)	93(11)	54(4)	25(3)	0	5(5)	0
T	0.0757(1)	0.16714(9)	0.22626(8)	0.77(2)	48(2)	20.7(8)	24.6(7)	0(1)	8(1)	-1.7(8)
M1	0	0	0.5	0.73(3)	48(4)	16(1)	27(1)	0	13(2)	0
M2	0	0.3332(1)	0.5	0.73(2)	39(2)	20.0(8)	24.7(8)	0	6(1)	0
A	0	0.5	0	2.50(5)	209(6)	73(2)	65(2)	0	25(3)	0
GFS15a (1M polytype)										
O1	0.0162(7)	0	0.1700(3)	2.10(8)	200(10)	49(4)	56.7(3)	0	9(5)	0
O2	0.3264(4)	0.2315(3)	0.1692(2)	2.21(6)	163(8)	78(3)	56(2)	-27(4)	39(3)	-4(2)
O3	0.1322(4)	0.1685(2)	0.3920(2)	1.75(5)	173(8)	51(2)	40(2)	2(4)	21(3)	0(2)
O4	0.1285(6)	0.5	0.3969(3)	1.75(7)	156(11)	58(4)	39(3)	0	24(5)	0
T	0.0758(1)	0.16694(9)	0.22642(8)	1.23(2)	85(2)	36.7(8)	38.7(7)	-1(1)	22(1)	1(7)
M1	0	0	0.5	1.18(3)	85(4)	28(1)	43(1)	0	28(2)	0
M2	0	0.3331(1)	0.5	1.13(2)	69(2)	30.6(9)	39.1(8)	0	18(1)	0
A	0	0.5	0	3.37(5)	283(6)	103(2)	86(2)	0	34.5(3)	0
H87 (1M polytype)										
O1	0.0160(6)	0	0.1705(3)	1.82(6)	199(10)	33(3)	49(3)	0	-1(4)	0
O2	0.3270(4)	0.2296(2)	0.1690(2)	1.86(4)	157(6)	53(2)	52(2)	-30(3)	29(3)	-7(2)
O3	0.1330(3)	0.1690(2)	0.3923(2)	1.39(4)	141(6)	30(2)	39(2)	-2(3)	12(2)	0(1)
O4	0.1263(5)	0.5	0.3970(3)	1.52(6)	126(8)	48(3)	37(2)	0	10(4)	0
T	0.0755(1)	0.16709(6)	0.22608(6)	0.88(1)	66(2)	12.4(5)	37.8(5)	0(1)	15.2(7)	-0.1(5)
M1	0	0	0.5	0.95(2)	67(2)	12.3(8)	43.1(9)	0	20(1)	0
M2	0	0.33309(7)	0.5	0.95(1)	63(2)	15.8(6)	40.5(6)	0	12.4(8)	0
A	0	0.5	0	2.74(4)	230(5)	69(2)	81(2)	0	23(2)	0

Table 5. Continued

Atom	x/a	y/b	z/c	B _{eq}	b ₁₁ [*]	b ₂₂ [*]	b ₃₃ [*]	b ₁₂ [*]	b ₁₃ [*]	b ₂₃ [*]
CC1 (1M polytype)										
O1	0.0156(7)	0	0.1710(3)	1.58(7)	160(10)	34(4)	37(3)	0	-10(5)	0
O2	0.3271(4)	0.2297(3)	0.1689(2)	1.63(5)	122(8)	60(3)	35(2)	-27(4)	21(3)	-6(2)
O3	0.1326(4)	0.1693(3)	0.3921(2)	1.11(4)	108(7)	36(2)	20(2)	-2(4)	-2(3)	0(2)
O4	0.1269(6)	0.5	0.3977(3)	1.21(7)	90(10)	51(4)	20(2)	0	0(4)	0
T	0.0757(1)	0.16710(9)	0.22650(7)	0.66(1)	47(2)	18.0(8)	19.2(6)	0(1)	6.0(9)	0.9(7)
M1	0	0	0.5	0.74(2)	50(4)	18(1)	25(1)	0	11(2)	0
M2	0	0.3334(1)	0.5	0.75(2)	41(2)	23.2(8)	22.1(7)	0	4(1)	0

A	0	0.5	0	2.61(4)	216(6)	74(2)	69(2)	0	20(3)	0
C3-31 (1M polytype)										
O1	0.0181(6)	0	0.1700(3)	1.59(7)	170(10)	26(3)	47(3)	0	9(5)	0
O2	0.3252(4)	0.2307(3)	0.1681(2)	1.59(5)	148(8)	49(3)	37(2)	-32(4)	22(3)	-7(2)
O3	0.1322(4)	0.1686(2)	0.3915(2)	1.19(4)	138(7)	28(2)	26(2)	-4(3)	8(3)	-1(2)
O4	0.1280(6)	0.5	0.3975(3)	1.33(7)	110(10)	44(4)	30(3)	0	9(4)	0
T	0.0756(1)	0.16706(8)	0.22573(7)	0.74(2)	70(2)	14.8(8)	23.3(7)	1(1)	7.7(9)	0.1(7)
M1	0	0	0.5	0.77(2)	64(3)	13(1)	30(1)	0	14(2)	0
M2	0	0.33325(9)	0.5	0.89(2)	63(2)	21.8(8)	29.7(7)	0	6(1)	0
A	0	0.5	0	2.74(4)	233(6)	73(2)	78(2)	0	26(3)	0
B1 (1M polytype)										
O1	0.0169(4)	0	0.1704(2)	1.67(5)	191(8)	34(2)	39(2)	0	-5(3)	0
O2	0.3256(3)	0.2313(2)	0.1685(2)	1.71(4)	125(5)	66(2)	39(1)	-35(2)	16(2)	-6(1)
O3	0.1326(3)	0.1687(2)	0.3919(1)	1.23(3)	116(4)	38(2)	26(1)	0(2)	4(2)	0(1)
O4	0.1268(4)	0.5	0.3978(2)	1.42(5)	101(6)	60(3)	26(2)	0	0(3)	0
T	0.0756(1)	0.16702(6)	0.22575(5)	0.78(1)	52(2)	22.5(5)	24.8(4)	0.6(8)	5.3(6)	0.3(4)
M1	0	0	0.5	0.80(1)	52(2)	19.1(7)	30.2(7)	0	11.3(9)	0
M2	0	0.33318(6)	0.5	0.91(1)	51(2)	27.8(6)	29.0(5)	0	4.8(6)	0
A	0	0.5	0	2.64(3)	212(4)	78(2)	71(1)	0	20(2)	0

Table 5. Continued

Atom	x/a	y/b	z/c	B _{eq}	b ₁₁ [*]	b ₂₂ [*]	b ₃₃ [*]	b ₁₂ [*]	b ₁₃ [*]	b ₂₃ [*]
C6c (2M ₁ polytype)										
O11	0.7424(4)	0.3147(2)	0.1645(1)	1.78(5)	158(9)	58(2)	9.6(4)	-30(4)	0(2)	3.2(8)
O21	0.2417(4)	0.3546(2)	0.1656(1)	1.82(5)	153(9)	64(2)	9.4(4)	23(4)	0(2)	-3.4(8)
O22	0.4327(4)	0.0846(2)	0.16571(8)	1.69(4)	226(8)	31(2)	9.1(4)	-3(4)	7(1)	0.0(8)
O31	0.4295(4)	0.2432(2)	0.05410(8)	1.31(4)	132(7)	37(2)	7.3(4)	-4(4)	0(1)	-0.1(8)
O32	0.9373(4)	0.4125(2)	0.05407(8)	1.41(4)	153(7)	40(2)	6.9(3)	11(5)	0(1)	-1.5(8)
O4	0.9364(4)	0.0739(2)	0.05117(8)	1.37(4)	174(8)	27(2)	7.5(3)	17(4)	2(1)	-5.0(7)
T1	0.4614(1)	0.25084(7)	0.13691(3)	0.93(1)	91(3)	22.0(6)	6.1(1)	2(1)	1.2(4)	-0.1(3)
T2	0.9628(1)	0.41783(8)	0.13689(3)	0.92(1)	81(2)	23.6(6)	6.5(1)	-3(2)	1.8(4)	0.2(3)
M1	0.75	0.25	0	0.93(1)	78(3)	21.3(6)	7.1(1)	-6(2)	2.5(4)	-0.7(3)
M2	0.2501(1)	0.08323(5)	0.00002(2)	0.92(1)	80(2)	21.2(4)	6.9(1)	-1(2)	1.0(3)	1.0(2)
A	0	0.0852(1)	0.25	2.87(2)	267(4)	79(1)	18.2(2)	0	4.6(7)	0
* anisotropic temperature factors b _{ij} are of the form exp [- (h ^{2b} ₁₁ +...+2hkb ₁₂ +...)].										

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