

TABLE 3. Refined atomic positions and displacement parameters (\AA^2) of monoclinic wairakite at selected pressures

	P_{amb}				0.9 GPa				2.1 GPa	
	x/a	y/b	z/c	U_{iso}	x/a	y/b	z/c	U_{iso}	x/a	y/b
T11A	0.1107(8)	0.1580(9)	0.4186(8)	0.020(1)	0.1050(8)	0.1555(9)	0.4175(8)	0.020(1)	0.107(1)	0.151(1)
T11B	0.8711(9)	0.3369(9)	0.4020(8)	0.020(1)	0.8683(9)	0.3404(9)	0.402(1)	0.020(1)	0.868(1)	0.339(1)
T12A	0.4231(8)	0.131(1)	0.1597(9)	0.020(1)	0.4285(9)	0.136(1)	0.1575(9)	0.020(1)	0.429(1)	0.130(1)
T12B	0.5984(8)	0.3721(9)	0.1688(8)	0.020(1)	0.6012(8)	0.374(1)	0.1698(9)	0.020(1)	0.595(1)	0.383(1)
T2A	0.1746(8)	0.4064(8)	0.1364(9)	0.020(1)	0.1790(9)	0.409(1)	0.1388(9)	0.020(1)	0.190(1)	0.407(1)
T2B	0.851(1)	0.0861(9)	0.1201(9)	0.020(1)	0.852(1)	0.085(1)	0.1207(9)	0.020(1)	0.859(1)	0.082(1)
O11A	0.100(1)	0.355(2)	0.2249(9)	0.020(1)	0.102(1)	0.358(2)	0.227(1)	0.022(2)	0.112(2)	0.353(2)
O11B	0.902(2)	0.153(1)	0.2153(8)	0.020(1)	0.912(2)	0.151(2)	0.2138(9)	0.022(2)	0.931(2)	0.119(2)
O12A	0.388(1)	0.142(2)	0.4638(9)	0.020(1)	0.387(1)	0.128(2)	0.4659(9)	0.022(2)	0.356(3)	0.125(2)
O12B	0.604(1)	0.357(2)	0.4835(9)	0.020(1)	0.603(2)	0.352(2)	0.481(1)	0.022(2)	0.606(2)	0.339(2)
O21A	0.201(1)	0.113(2)	0.358(1)	0.020(1)	0.196(1)	0.115(2)	0.354(1)	0.022(2)	0.189(1)	0.121(2)
O21B	0.775(1)	0.401(2)	0.378(2)	0.020(1)	0.775(1)	0.409(2)	0.376(2)	0.022(2)	0.761(1)	0.390(2)
O22A	0.134(2)	0.461(1)	0.389(2)	0.020(1)	0.127(2)	0.460(1)	0.387(2)	0.022(2)	0.136(2)	0.455(1)
O22B	0.838(1)	0.0323(9)	0.358(2)	0.020(1)	0.824(1)	0.035(1)	0.344(2)	0.022(2)	0.821(1)	0.033(1)
O31A	0.390(2)	0.2249(9)	0.096(2)	0.020(1)	0.403(2)	0.2261(9)	0.084(1)	0.022(2)	0.414(2)	0.231(1)
O31B	0.648(1)	0.278(1)	0.118(1)	0.020(1)	0.645(2)	0.275(1)	0.123(2)	0.022(2)	0.638(2)	0.275(1)
O32A	0.4864(9)	0.385(2)	0.134(2)	0.020(1)	0.494(1)	0.397(1)	0.122(2)	0.022(2)	0.496(1)	0.409(2)
O32B	0.5406(8)	0.125(2)	0.165(1)	0.020(1)	0.5449(9)	0.114(2)	0.164(2)	0.022(2)	0.546(1)	0.101(2)
M2*	0.0157(7)	0.245(1)	0.120(1)	0.049(3)	0.0160(7)	0.242(1)	0.1180(9)	0.041(3)	–.003(2)	0.251(3)
M12B†	0.75	0.396(6)	0.00	0.040	0.75	0.377(7)	0.00	0.040	0.75	0.36(2)
WA	0.141(2)	0.119(2)	0.142(2)	0.057(5)	0.144(2)	0.124(2)	0.141(2)	0.038(6)	0.146(4)	0.134(5)
WB	0.899(2)	0.368(2)	0.118(2)	0.057(5)	0.906(2)	0.379(2)	0.123(2)	0.038(6)	0.891(4)	0.365(5)

Note: Values in italics correspond to structural parameters not refined during the fit procedure.

* Occupancy factor for M2 is 0.91, 0.92, 0.92, 0.94 for GPa P_{amb} 0.9, 2.1 GPa, $P_{\text{amb}}(\text{rev})$, respectively.

† Occupancy factor for M12B is 0.28 GPa for all the refinements.

TABLE 4. T-O framework distances and coordination distances ($<3.15 \text{\AA}$) of the extra-framework species for selected refinements of monoclinic wairakite

	P_{amb}	0.9 GPa	2.1 GPa	$P_{\text{amb}}(\text{rev})$		P_{amb}	0.9 GPa	2.1 GPa	$P_{\text{amb}}(\text{rev})$
T11A-O12A	1.611(2)	1.611(2)	1.622(7)	1.611(2)	T12B-O11B	1.611(2)	1.612(2)	1.621(7)	1.610(2)
T11A-O21A	1.610(2)	1.610(2)	1.628(7)	1.611(2)	T12B-O22B	1.610(2)	1.610(2)	1.632(7)	1.610(2)
T11A-O31A	1.611(2)	1.611(2)	1.624(7)	1.611(2)	T12B-O31B	1.610(2)	1.610(2)	1.619(7)	1.611(2)
T11A-O32A	1.610(2)	1.610(2)	1.620(7)	1.610(2)	T12B-O32A	1.611(2)	1.610(2)	1.617(7)	1.610(2)
mean	1.610	1.610	1.623	1.620	mean	1.610	1.610	1.622	1.620
T11B-O12B	1.611(2)	1.611(2)	1.622(7)	1.611(2)	T2A-O11A	1.730(2)	1.730(2)	1.716(8)	1.731(2)
T11B-O21B	1.610(2)	1.610(2)	1.618(7)	1.610(2)	T2A-O12A	1.731(2)	1.730(2)	1.702(7)	1.730(2)
T11B-O31B	1.610(2)	1.610(2)	1.623(7)	1.610(2)	T2A-O21A	1.730(2)	1.730(2)	1.708(7)	1.731(2)
T11B-O32B	1.610(2)	1.610(2)	1.630(7)	1.611(2)	T2A-O22B	1.730(2)	1.730(2)	1.711(8)	1.730(2)
mean	1.610	1.610	1.623	1.620	mean	1.730	1.730	1.709	1.730
T12A-O11A	1.611(2)	1.611(2)	1.631(7)	1.611(2)	T2B-O11B	1.730(2)	1.731(2)	1.711(8)	1.730(2)
T12A-O22A	1.610(2)	1.610(2)	1.630(7)	1.611(2)	T2B-O12B	1.730(2)	1.730(2)	1.715(7)	1.731(2)
T12A-O31A	1.611(2)	1.611(2)	1.624(7)	1.610(2)	T2B-O21B	1.730(2)	1.730(2)	1.704(8)	1.730(2)
T12A-O32B	1.611(2)	1.610(2)	1.628(7)	1.611(2)	T2B-O22A	1.730(2)	1.730(2)	1.717(7)	1.731(2)
mean	1.611	1.610	1.628	1.620	mean	1.730	1.730	1.712	1.730
M2-O11A	2.36(2)	2.44(3)	2.56(4)	2.45(6)	M12B-O22B	2.48(4)	2.62(5)	2.7(1)	2.70(9)
M2-O11B	2.38(2)	2.28(2)	2.39(4)	2.59(6)	M12B-O22B	2.48(4)	2.62(5)	2.7(1)	2.70(9)
M2-O12A	2.33(3)	2.48(3)	2.82(4)	2.53(6)	M12B-O31B	2.68(5)	2.59(6)	2.7(1)	2.9(1)
M2-O12B	2.56(2)	2.44(2)	2.23(3)	2.33(5)	M12B-O31B	2.68(5)	2.59(6)	2.7(1)	2.9(1)
M2-O31A		2.94(2)	2.97(4)		M12B-WB	2.62(3)	2.67(2)	2.51(5)	2.69(8)
M2-WA	2.45(3)	2.38(3)	2.58(7)	2.40(6)	M12B-WB	2.62(3)	2.67(2)	2.51(5)	2.69(8)
M2-WB	2.32(2)	2.38(2)	2.11(7)	2.46(5)					
WA-O11B			3.06(6)		WB-O11A	3.10(4)	3.00(3)		2.98(8)
WA-O21A	3.03(3)	2.93(3)	2.60(6)	2.94(7)	WB-O12A	3.13(3)	3.06(3)		
WA-O21B		3.14(3)			WB-O32B	3.04(4)	2.93(3)	2.86(7)	2.89(9)