

TABLE 3. (on deposit). Crystal and structure refinement data of tsilaisite.

a (Å)	15.9461(5)	
c	7.1380(3)	
V (Å ³)	1571.9(1)	
Space group	$R3m$	
Z	3	
D_{calc} (g cm ⁻³)	3.133	
Radiation	MoK α	
Monochromator	graphite	
Set of measured reflections	1682	
	Standard*	Split-site SREF*
$wR2$ (%)	5.16	4.90
$R1$ (%) for $I_o > 2\sigma(I_o)$	2.05	1.91
$R1$ (%) for all reflections	2.12	1.97
GooF	1.122	1.135
Extinction coefficient	0.0071(3)	0.0070(3)
Flack parameter	0.13(2)	0.13(2)
Larg. diff. peak-hole (e Å ⁻³)	1.19 and -0.45	0.37 and -0.53

*Standard and Split-site SREF denote, respectively, structural refinements carried out with the O1 site at (0,0, z) and the O2 site at (x ,2 x , z), and with O1 at (x ,2 x , z) and O2 at (x , y , z) to allow for positional disorder, as indicated by the high U_{eq} values (Burns *et al.*, 1994).

TABLE 4. (on deposit). Final fractional atomic coordinates and equivalent displacement parameters (\AA^2).

Site	Standard*				Split-site SREF*			
	x	y	z	U_{eq}	x	y	z	U_{eq}
X	0	0	0.22856(40)	0.0269(8)	0	0	0.22897(37)	0.0261(8)
Y	0.12399(4)	$x/2$	0.62408(9)	0.0113(1)	0.12400(4)	$x/2$	0.62407(8)	0.0114(1)
Z	0.29803(3)	0.26129(3)	0.61115(7)	0.0060(1)	0.29801(3)	0.26127(3)	0.61120(3)	0.0060(1)
B	0.10993(8)	$2x$	0.45431(29)	0.0067(3)	0.10999(7)	$2x$	0.45429(27)	0.0070(3)
T	0.19190(2)	0.18997(3)	0	0.00479(8)	0.19191(2)	0.18997(2)	0	0.00470(8)
O1	0	0	0.77938(51)	0.044(1)	0.02087(23)	$x/2$	0.77961(47)	0.0078(8)†
O2	0.06139(6)	$2x$	0.48181(26)	0.0197(4)	0.07115(16)	0.12293(12)	0.48192(23)	0.0101(4)†
O3	0.26843(13)	$x/2$	0.51001(22)	0.0115(3)	0.26862(12)	$x/2$	0.51004(20)	0.0114(2)
O4	0.09351(6)	$2x$	0.07011(21)	0.0085(2)	0.09348(5)	$2x$	0.07006(19)	0.0082(2)
O5	0.18698(11)	$x/2$	0.09173(20)	0.0084(2)	0.18697(10)	$x/2$	0.09176(19)	0.0083(2)
O6	0.19732(7)	0.18723(7)	0.77527(15)	0.0079(2)	0.19727(7)	0.18721(7)	0.77531(14)	0.0079(2)
O7	0.28539(7)	0.28583(7)	0.08002(14)	0.0063(2)	0.28533(7)	0.28581(6)	0.08008(13)	0.0062(2)
O8	0.21011(7)	0.27092(8)	0.44140(15)	0.0080(2)	0.21009(7)	0.27095(7)	0.44150(14)	0.0078(2)
H3	0.2594(27)	$x/2$	0.4005(51)	0.01720†	0.2559(24)	$x/2$	0.4085(48)	0.01706†

* Standard and Split-site SREF as in Table 3.

† Isotropic displacement parameter; for H3 was constrained to $1.5U_{eq}(O3)$

TABLE 5. (on deposit). Anisotropic displacement parameters (\AA^2) of tsilaisite.

Site	Standard*						Split-site SREF*					
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
X	0.030(1)	0.030(1)	0.021(1)	0	0	0.0149(5)	0.029(1)	0.029(1)	0.021(1)	0	0.00	0.0143(5)
Y	0.0108(2)	0.0080(2)	0.0160(2)	-0.0013(1)	-0.0026(2)	0.0054(1)	0.0108(2)	0.0081(2)	0.0162(2)	-0.0013(1)	-0.0027(1)	0.0054(1)
Z	0.0063(2)	0.0073(2)	0.0047(2)	0.0005(1)	-0.0001(1)	0.0035(1)	0.0063(2)	0.0072(2)	0.0046(2)	0.0006(1)	-0.0001(1)	0.0035(1)
B	0.0072(5)	0.0059(7)	0.0065(7)	0.0003(6)	0.0002(3)	0.0029(4)	0.0074(5)	0.0071(7)	0.0063(6)	0.0002(5)	0.0001(3)	0.0035(4)
T	0.0045(2)	0.0048(1)	0.0046(1)	-0.0004(1)	-0.0000(1)	0.0029(1)	0.0048(1)	0.0047(1)	0.0046(1)	-0.0004(1)	0.0000(1)	0.0023(1)
O1	0.064(2)	0.064(2)	0.005(1)	0	0	0.032(1)	0	0	0	0	0	0
O2	0.0305(8)	0.0060(6)	0.0144(7)	0.0005(5)	0.0003(3)	0.0030(3)	0	0	0	0	0	0
O3	0.0237(8)	0.0104(4)	0.0047(5)	-0.0003(3)	-0.0006(5)	0.0119(4)	0.0235(7)	0.0105(4)	0.0044(5)	-0.0003(2)	-0.0005(5)	0.0118(4)
O4	0.0069(4)	0.0125(6)	0.0079(5)	-0.0013(5)	-0.0007(2)	0.0063(3)	0.0068(4)	0.0116(6)	0.0078(5)	-0.0013(4)	-0.0006(2)	0.0058(3)
O5	0.0142(6)	0.0066(4)	0.0071(5)	0.0009(2)	0.0018(5)	0.0071(3)	0.0145(6)	0.0064(3)	0.0067(5)	0.0007(2)	0.0014(4)	0.0072(3)
O6	0.0088(4)	0.0095(4)	0.0043(3)	-0.0004(3)	0.0007(3)	0.0038(3)	0.0087(4)	0.0096(4)	0.0041(3)	-0.0007(3)	0.0004(3)	0.0037(3)
O7	0.0061(4)	0.0053(4)	0.0052(4)	-0.0006(3)	0.0005(3)	0.0013(3)	0.0058(3)	0.0054(3)	0.0053(3)	-0.0006(3)	0.0005(3)	0.0013(3)
O8	0.0064(4)	0.0116(4)	0.0073(4)	0.0027(3)	0.0005(3)	0.0055(3)	0.0063(4)	0.0115(4)	0.0069(3)	0.0027(3)	0.0006(3)	0.0055(3)

* Standard and Split-site SREF as in Table 3.

TABLE 6. (on deposit). Relevant bond distances (Å), and mean atomic numbers (m.a.n.) of tsilaisite

	Standard*	Split-site SREF*		
B-O2	1.3551(27)	1.3634(26)		
B-O8 ($\times 2$)	1.3867(15)	1.3854(14)		
<B-O>	1.376	1.378		
m.a.n. B	5	5		
T-O4	1.6250(6)	1.6250(5)		
T-O5	1.6373(7)	1.6374(6)		
T-O7	1.6145(10)	1.6140(9)		
T-O6	1.6082(10)	1.6078(10)		
<T-O>	1.621	1.621		
m.a.n. T	14	14		
X-O2 ($\times 3$)	2.4784(27)	2.4831(24)		
X-O4 ($\times 3$)	2.8195(19)	2.8020(18)		
X-O5 ($\times 3$)	2.7607(18)	2.7616(17)		
<X-O>	2.686	2.682		
m.a.n. X	8.36(9)	8.30(8)		
		Y1	Y2	Y3
Y-O1	2.0398(20)	2.1776(24)	2.1776(24)	1.8058(33)
Y-O2	1.9836(12)	1.8715(20)	2.1021(21)	1.8715(20)
Y-O2	1.9836(12)	2.1021(21)	2.1021(21)	1.8715(20)
Y-O3	2.1545(18)	2.1566(17)	2.1566(17)	2.1566(17)
Y-O6	2.0456(11)	2.0455(10)	2.0455(10)	2.0455(10)
Y-O6	2.0456(11)	2.0455(10)	2.0455(10)	2.0455(10)
<Y-O>	2.042	2.071	2.117	1.950
m.a.n. Y	16.46(5)	16.56(4)		
Z-O3	1.9732(8)	1.9725(9)		
Z-O6	1.8572(11)	1.8575(9)		
Z-O8	1.9163(11)	1.9166(10)		
Z-O7	1.9573(10)	1.9582(9)		
Z-O7'	1.8786(10)	1.8797(9)		
Z-O8'	1.8828(11)	1.8828(10)		
<Z-O>	1.911	1.911		
m.a.n. Z	13.22(5)	13.23(4)		

*Standard and Split-site SREF as in Table 3.