Table OM1. Data collection and structure refinement details for gungerite.

Diffractometer	SuperNova Rigaku micro-diffractometer
X-ray radiation	Mo*K*α (λ = 0.71075 Å)
Temperature	286 K
Chemical formula	$TlAs_{5.293}Sb_{3.707}S_{13}$
Space group	*Pbcn*
Unit cell dimensions	*a* = 20.1958(3) Å
	b = 11.5258(2) Å
	c = 20.1430(2) Å
V	4688.74(12) Å^3
Z	8
$\rho_{calc.}$ (for above formula)	4.162 g·cm^{-3}
Absorption coefficient	19.633 mm^{-1}
F(000)	5222
Crystal size	0.28 × 0.18 × 0.11 mm
θ range	4.53 to 27.75°
Index ranges	$-26 \le h \le 26$, $-14 \le k \le 14$, $-26 \le l \le 26$
Reflections collected/unique	114573/5652; R_{int} = 0.0716
Reflections with $I > 3\sigma I$	4790
Completeness to θ = 27.75°	97%
Refinement method	Full-matrix least-squares on F^2
Parameters/restraints	214/0
GoF	1.82
Final *R* indices [$I > 3\sigma(I)$]	R_1 = 0.0373, wR_2 = 0.1213
R indices (all data)	R_1 = 0.0501, wR_2 = 0.1266
Weighting scheme, weights	Weighting scheme based on measured s.u.'s; $w = 1/(\sigma^2(I) + 0.0025I^2)$
Largest diff. peak/hole	+1.38/–1.31 *e*·Å^{-3}
Twin matrix; Tw_{vol1}/Tw_{vol2}	$\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$; 0.8354(9)/0.1646(9)

Table OM2. Atom coordinates, equivalent displacement parameters (in Å^2) and occupational factors (Occ.) for gungerite.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}	*Occ.*
Tl1	0.24226(3)	0.20605(5)	0.50810(3)	0.03918(18)	
Sb1	0.39295(4)	0.12605(7)	0.66069(4)	0.0250(2)	
Sb2/Sb2’	0.07501(4)	0.40811(8)	0.45577(5)	0.0283(3)	0.840(12)Sb/0.160(12)As
Sb3/Sb3’	0.29719(4)	0.38533(7)	0.68080(4)	0.0276(3)	0.844(13)Sb/0.156(13)As
Sb4/Sb4’	0.09147(4)	0.16104(7)	0.35455(4)	0.0257(3)	0.781(11)Sb/0.219(11)As
As1/As1’	0.43140(5)	0.37921(10)	0.55607(5)	0.0247(4)	0.820(12)As/0.180(12)Sb
As2/As2’	0.20330(5)	0.40234(10)	0.32389(6)	0.0226(4)	0.938(12)As/0.062(12)Sb
As3	0.35761(6)	0.30182(9)	0.39780(6)	0.0222(3)	
As4	0.43974(6)	0.25441(10)	0.31259(6)	0.0247(3)	
As5	0.39823(6)	0.21156(10)	0.15027(6)	0.0248(3)	
S1	0.41390(14)	0.3368(3)	0.70323(14)	0.0246(8)	
S2	0.41286(14)	0.1821(3)	0.54310(14)	0.0235(8)	
S3	0.34058(14)	0.0806(2)	0.09520(15)	0.0271(8)	
S4	0.08958(15)	0.2036(3)	0.47605(15)	0.0252(8)	
S5	0.27333(14)	0.1806(3)	0.66270(15)	0.0245(8)	
S6	0.37608(16)	0.1333(3)	0.25265(16)	0.0319(9)	
S7	0.49909(15)	0.1287(3)	0.12794(16)	0.0311(9)	
S8	0.20989(14)	0.2062(2)	0.33975(15)	0.0233(8)	
S9	0.32377(15)	0.4411(3)	0.56535(16)	0.0291(9)	
S10	0.31644(15)	0.4279(3)	0.32216(16)	0.0277(9)	
S11	0.19030(16)	0.4640(3)	0.43110(16)	0.0312(9)	
S12	0.05423(14)	0.3589(2)	0.33641(14)	0.0247(8)	
S13	0.43602(15)	0.4168(3)	0.44297(14)	0.0269(8)	