Revision 2

Lead–tellurium oxysalts from Otto Mountain near Baker, California: VIII. Fuettererite, $Pb_3Cu^{2+}_6Te^{6+}O_6(OH)_7Cl_5$, a new mineral with double spangolite–type sheets.

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ABSTRACT

Fuettererite, $Pb_3Cu^{2+}_6Te^{6+}O_6(OH)_7Cl_5$, is a new tellurate from Otto Mountain near Baker, California, named for Otto Fuetterer who is largely responsible for the development of the mining claims on Otto Mountain. The new mineral is known from only two specimens, one from the NE2 vein and the other from the Bird Nest drift. Fuettererite occurs in vugs in quartz, on the first specimen associated with Br-rich chlorargyrite, iodargyrite, and telluroperite and on the second specimen associated with anglesite, anatacamite, atacamite, chalcopyrite, galena, goethite, hematite, muscovite, phosphohedyphane, timroseite, and wulfenite. It is interpreted as having

formed from the partial oxidation of primary sulfides and tellurides during or following brecciation of quartz veins. Fuettererite is hexagonal, space group *R*-3, $a = 8.4035(12)$, $c = 44.681(4)$ Å, $V = 2732.6(6)$ Å^3 and $Z = 6$. Crystals are tabular to short prismatic, exhibit the forms {100}, {101}, and {001} and reach a maximum dimension of 50 μm. The color is bluish green, the streak is pale bluish-green, and the luster is adamantine. The Mohs hardness is estimated at between 2 and 3. The new mineral is brittle with irregular fracture and one perfect cleavage on {001}. The calculated density based on the empirical formula is 5.528 g/cm^3. Fuettererite is uniaxial (–), with calculated indices of refraction of $\omega = 2.04$ and $\varepsilon = 1.97$, and is dichroic bluish-green, $E < O$. Electron microprobe analysis provided: PbO 41.45, CuO 30.35, Al_2O_3 0.23, TeO_3 12.80, Cl 12.08, H_2O 3.55 (structure), O=Cl -2.73, total 97.73 wt%. The empirical formula (based on 18 O + Cl atoms *pfu*) is: $Pb_{2.88}Cu^{2+}_{5.92}Al_{0.07}Te^{6+}_{1.13}O_{6.59}(OH)_{6.12}Cl_{5.29}$. The ten strongest powder X-ray diffraction lines are [d_{obs} in Å (*hkl*) *I*]: 6.106 (104) 44, 3.733 (0·0·12) 100, 2.749 (12-1) 53, 2.6686 (12-4) 49, 2.5289 (12-7) 41, 2.2772 (1·2·11) 38, 1.9637 (315, 1·2·-16) 87, 1.8999 (multiple) 48, 1.5976 (multiple) 40, and 1.5843 (410, 1·2·23, 143) 44. The crystal structure of fuettererite ($R_1 = 0.031$ for 971 reflections with $F_o > 4\sigma F$) contains edge-sharing sheets of CuO_5Cl and TeO_6 octahedra. These sheets are virtually identical to that in the structure of spangolite, but in fuettererite they are linked together to form a double sheet. The double octahedral sheets alternate with thick double layers of PbO_2Cl_6 polyhedra. The CuO_5Cl octahedra exhibit pronounced Jahn-Teller distortions and the PbO_2Cl_6 polyhedron has a lopsided distribution of bond lengths attributable to the localization of the Pb^{2+} $6s^2$ lone-pair electrons.

Keywords: Fuettererite; new mineral; tellurate; crystal structure; spangolite; Pb^{2+} $6s^2$ lone-pair; Otto Mountain, California.

INTRODUCTION

During the course of continuing investigations of the remarkable secondary mineral assemblage at Otto Mountain, near Baker, California (Housley et al. 2011), we have thus far described eight new Pb–Te oxysalts: ottoite, housleyite, thorneite, markcooperite, timroseite, paratimroseite, telluroperite, and chromscheffelinite (see Table 1), and have reported the structure determination of munakataite (Kampf et al. 2010g). In this contribution, we describe fuettererite and in the accompanying paper we describe agaite (Kampf et al. 2012b), the ninth and tenth new Pb–Te oxysalt minerals from this deposit.

The new mineral is named fuettererite in honor of Otto Fuetterer (born *ca*. 1880; died *ca*. 1970), who is largely responsible for the development of the mining claims on Otto Mountain. In 1940, Fuetterer, a naturalized American citizen born in Germany and then about 60 years old, filed six claims on the hill named Good Hope 1–6. The following year a friend of his, A. G. Andrews (AGA), filed 18 adjacent claims named Aga 1–18; in 1942 Andrews added two more, Aga 19 and 20. They held these claims together until sometime after 1950 when Fuetterer became sole owner of all 26 claims. According to Lois Clark, Baker resident and longtime friend of Fuetterer, he was a well-educated man and had an appreciation and understanding of the sciences. He continued to live on and work the claims until near the time of his death around 1970. During the time he lived on the mountain, originally named "Hopeless Hill", people in Baker came to call it Otto Mountain and that name, and the name Aga mine stuck when the U. S. Geological Survey produced their latest series of maps. It is worth noting that the new mineral ottoite was named for the locality, rather than for Otto Fuetterer.

The new mineral and name has been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2011–111). One holotype and one cotype specimen are deposited in the Natural History Museum of Los Angeles County, catalogue number 63588 and 64589, respectively.

OCCURRENCE

The holotype specimen of fuettererite was found at a small prospect in a quartz vein referred to as the NE2 vein (35.27776°N, 116.09331°W, elevation 1090 feet) on the northeast flank of Otto Mountain, about 0.4 miles north of the Aga mine. The cotype specimen is from the Bird Nest drift (35.27677°N, 116.09927°W) on the southwest flank of Otto Mountain, 0.4 miles northwest of the Aga mine.

Fuettererite is very rare. It has been found on only two specimens. The holotype specimen was found by two of the authors (RMH and JM). On this specimen, about 10 crystals of the mineral occur scattered in a vug in quartz closely associated with Br-rich chlorargyrite, iodargyrite, and telluroperite. The cotype specimen was found by Jerry A. Baird of Lake Havasu City, Arizona. On this specimen, tiny fuettererite crystals occur intergrown with paratacamite in vugs in quartz. Other minerals that occur on this specimen include anglesite, anatacamite, atacamite, chalcopyrite, galena, goethite, hematite, muscovite, phosphohedyphane, timroseite, and wulfenite. Other species identified in the mineral assemblages at Otto Mountain include acanthite, agaite, boleite, brochantite, burckhardtite, calcite, caledonite, celestine, cerussite, chromschieffelinite, chrysocolla, devilline, diaboleite, eztlite, fluorite, fornacite, gold, hessite, housleyite, jarosite, khinite, kuranakhite, linarite, malachite, markcooperite, mimetite,

mottramite, munakataite, murdochite, ottoite, paratimroseite, perite, plumbojarosite, pyrite, thorneite, vanadinite, and vauquelinite.

Fuettererite occurs as a secondary oxidation zone mineral and is presumed to have formed by oxidation of tellurides, chalcopyrite and galena. Additional background on the occurrence is provided in Kampf et al. (2010a) and Housley et al. (2011).

PHYSICAL AND OPTICAL PROPERTIES

On the holotype specimen, the mineral occurs as thick tabular to short prismatic crystals up to about 50 μm in maximum dimension and exhibiting the forms {100} and {001}. On the cotype specimen, fuettererite occurs as tablets up to about 10 μm in diameter and 2 μm thick and exhibiting the forms {101} and {001} (Figs. 1 and 2). No twinning was observed optically under crossed polars or based upon single-crystal X-ray diffraction. The color is bluish green, the streak is pale bluish green, and the luster is adamantine. The Mohs hardness could not be measured, but is estimated to be between 2 and 3. The new mineral is brittle with irregular fracture and one perfect cleavage on {001}. The density could not be measured because it is greater than those of available high-density liquids and there is insufficient material for physical measurement. The calculated density based on the empirical formula is 5.528 g/cm^3 and that based on the ideal formula is 5.552 g/cm^3. Fuettererite is readily soluble in cold dilute HCl.

Crystals of fuettererite are uniaxial (–) with the indices of refraction $\omega = 2.04$ and $\varepsilon = 1.97$, calculated from the retardation = 0.07 (measured with a Berek compensator) and $n_{av} = 2.015$ (based upon the Gladstone–Dale relationship). The mineral is dichroic bluish green, $E < O$.

CHEMICAL COMPOSITION

Quantitative chemical analyses of fuettererite were performed using a JEOL8200 electron microprobe (WDS mode, 15 kV, 5 nA, 1 μm beam diameter) at the Division of Geological and Planetary Sciences, California Institute of Technology. The standards used were: galena (for Pb), cuprite (for Cu), anorthite (for Al), Sb_2Te_3 (for Te), and sodalite (for Cl). Analytical results are given in Table 2. No other elements were detected in EDS analyses. There was insufficient material for CHN analyses, so H_2O was calculated on the basis of 10 total cations (Pb + Cu + Al + Te), charge balance and 18 total anions (O + Cl) *pfu*, as determined by the crystal structure analysis (see below). Note that fuettererite is prone to electron beam damage, which contributes to the low analytical total. This is a common feature observed in most secondary tellurate species (e.g. Kampf et al. 2010a–e; Kampf et al. 2012a,b; Mills et al. 2009, 2010).

The empirical formula (based on 18 O + Cl atoms *pfu*) is: $Pb_{2.88}Cu^{2+}_{5.92}Al_{0.07}Te^{6+}_{1.13}O_{6.59}(OH)_{6.12}Cl_{5.29}$. The simplified formula is $Pb_3Cu^{2+}_6Te^{6+}O_6(OH)_7Cl_5$, which requires PbO 43.97, CuO 31.34, TeO_3 11.53, Cl 11.64, H_2O 4.14, O=Cl –2.63, total 100 wt%.

X-RAY CRYSTALLOGRAPHY AND STRUCTURE DETERMINATIONS

All powder and single-crystal X-ray diffraction data were obtained on a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer utilizing monochromatized Mo*K*α radiation. Observed powder *d*-values (with standard deviations) and intensities were derived by profile fitting using JADE 9.3 software. Data (in Å) are given in Table 3. Unit cell parameters refined from the powder data using JADE 9.3 with whole pattern fitting are: $a = 8.401(5)$, $c = 44.68(3)$ Å, and $V = 2731(3)$ Å^3. The observed powder data fit well with those calculated from the structure, also

using JADE 9.3. The relatively low precision of the cell refined from the powder data is attributable to the use of Mo*K*α radiation.

The Rigaku CrystalClear software package was used for processing of the diffraction data, including the application of an empirical multi-scan absorption correction using ABSCOR (Higashi 2001). The structure was solved by direct methods using SIR2004 (Burla et al. 2005). SHELXL-97 software (Sheldrick 2008) was used for the refinement of the structure. H atom positions were located in difference Fourier maps and were constrained to H–O distances of 0.90(3) Å with isotropic displacement parameters (×1.2) tied to those of the O atoms to which they are associated. Attempts to refine the occupancies of the cation sites indicated all to be very close to fully occupied and did not improve the value of R_1 substantially (0.0304 *vs* 0.0307); therefore, we report the refinement with all sites fully occupied and consistent with the ideal formula. Details concerning data collection and structure refinement are provided in Table 4. Fractional coordinates and atom displacement parameters are provided in Table 5, selected interatomic distances in Table 6 and bond valences in Table 7.

DESCRIPTION OF THE STRUCTURE

The structure (Fig. 3) contains edge-sharing sheets of CuO_5Cl and TeO_6 octahedra parallel to {001}. The two independent CuO_5Cl octahedra exhibit pronounced Jahn-Teller distortions with particularly long apical Cu–Cl distances. Each CuO_5Cl octahedron is associated with equivalent octahedra in an edge-sharing trimer lying on a threefold axis, with Cl as the common vertex. The Cl vertex extends significantly out of the plane of the sheet, where it also participates as a shared corner with an equivalent trimer in an adjacent sheet. This linkage, along with hydrogen bonds, serves to create double octahedral sheets (Fig. 4). The double octahedral sheets

alternate along **c** with thick double layers of PbO_2Cl_6 polyhedra. The PbO_2Cl_6 polyhedron has a lopsided distribution of bond lengths attributable to the localization of the Pb^{2+} $6s^2$ lone-pair electrons (Fig. 5).

The octahedral sheet is virtually identical to that in the structure of spangolite, $Cu_6Al(SO_4)(OH)_{12}Cl{\cdot}3H_2O$, except that in spangolite it is composed of CuO_5Cl, CuO_6 and AlO_6 octahedra (Figs. 3 and 6). The structures also differ in that spangolite has only single octahedral sheets and the common vertex of each Cu octahedral trimer links to a SO_4 tetrahedron. In the spangolite structure, SO_4 and H_2O groups rather than Pb polyhedra occur between the octahedral sheets and the sheets are linked to one another only via hydrogen bonding (Fig. 4).

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230

231 FIGURE CAPTIONS

232

233 Figure 1. SEM image of fuettererite tablets on the cotype specimen.

234

235 Figure 2. Crystal drawings (clinographic projections) of fuettererite showing prismatic (left) and
236 tabular (right) habits.

237

238 Figure 3. Structures of fuettererite (left) and spangolite (right) viewed down [110] with *c* vertical.
239 Unit cells are shown as dashed lines.

240

241 Figure 4. Detail of layers in fuettererite structure with Pb coordination shown in "ball–and–stick"
242 style..Hydrogen bonds are shown as single black lines.

243

244 Figure 5. Pb coordination in fuettererite. The lopsided distributions of bond lengths are
245 attributable to the localization of the lone-pair electrons. Bond lengths are given in Å.

246

247 Figure 6. Octahedral sheets in the structures of fuettererite (top) and spangolite (bottom), in both
248 cases viewed down **c**.

249

250 Table 1. New minerals described from Otto Mountain.

Mineral	Ideal Formula	Reference
Ottoite	$Pb_2Te^{6+}O_5$	Kampf et al. (2010a)
Housleyite	$Pb_6Cu^{2+}Te^{6+}_4O_{18}(OH)_2$	Kampf et al. (2010b)
Thorneite	$Pb_6(Te^{6+}_2O_{10})(CO_3)Cl_2(H_2O)$	Kampf et al. (2010c)
Markcooperite	$Pb_2(UO_2)Te^{4+}O_6$	Kampf et al. (2010d)
Timroseite	$Pb_2Cu^{2+}_5(Te^{6+}O_6)_2(OH)_2$	Kampf et al. (2010e)
Paratimroseite	$Pb_2Cu^{2+}_4(Te^{6+}O_6)_2(H_2O)_2$	Kampf et al. (2010e)
Telluroperite	$Pb_3Te^{4+}O_4Cl_2$	Kampf et al. (2010f)
Chromschieffelinite	$Pb_{10}Te^{6+}_6O_{20}(CrO_4)(H_2O)_5$	Kampf et al. (2012a)
Fuettererite	$Pb_3Cu^{2+}_6Te^{6+}O_6(OH)_7Cl_5$	This study
Agaite	$Pb_3Cu^{2+}Te^{6+}O_5(OH)_2(CO_3)$	Kampf et al. (2012b)

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252

253 Table 2. Chemical analytical data for fuettererite.

Constituent	Analysis 1	Analysis 2	Average
PbO	41.4(7)	41.5(7)	41.45
CuO	30.1(2)	30.6(3)	30.35
Al_2O_3	0.29(6)	0.17(6)	0.23
TeO_3	12.5(3)	13.1(3)	12.80
Cl	12.54(10)	11.62(10)	12.08
H_2O	3.42	3.68	3.55
O=Cl	–2.83	–2.62	–2.73
Total	97.42	98.05	97.73

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255

Table 3. X-ray powder diffraction data for fuettererite.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	$h\ k\ l$
7	14.81(5)	14.8937	11	0 0 3
		7.4468	5	0 0 6
23	7.18(3)	7.1830	8	1 0 1
4	6.912(15)	6.9198	9	0 1 2
44	6.106(3)	6.0977	32	1 0 4
9	5.641(11)	5.6430	7	0 1 5
10	4.973(9)	4.9646	3	0 0 9
9	4.427(6)	4.4308	6	0 1 8
10	4.196(4)	4.2018	6	1 1 0
47	4.0432(10)	4.0439	36	1 1 -3
100	3.733(5)	3.7234	100	0 0 12
27	3.697(5)	3.6594	30	1 1 -6
47	3.650(19)	3.6268	11	0 2 1
28	3.4575(14)	3.4599	22	0 2 4
29	3.3713(9)	3.3701	27	2 0 5
23	3.212(3)	3.2073	26	1 1 9
29	3.171(3)	3.1612	22	0 2 7
20	3.0488(12)	3.0488	23	2 0 8
14	2.976(5)	2.9787	10	0 0 15
		2.9228	4	0 1 14
22	2.7902(14)	2.7867	22	1 1 -12
53	2.749(5)	2.7455	40	1 2 -1
10	2.729(2)	2.7301	8	2 1 -2
49	2.6686(7)	2.6709	39	1 2 -4
26	2.6275(10)	2.6290	26	1 2 5
41	2.5289(15)	2.5261	48	1 2 -7
22	2.511(3)	2.4986	11	0 2 13
13	2.478(6)	2.4720	2	0 1 17
		2.4677	6	1 2 8
8	2.435(3)	2.4300	11	1 1 -15
12	2.416(5)	2.4259	5	3 0 0
		2.3994	3	2 0 14
		2.3943	2	0 3 3
5	2.3363(6)	2.3424	6	2 1 10
38	2.2772(8)	2.2776	28	1 2 11
11	2.2150(12)	2.2154	11	0 2 16
26	2.1372(3)	2.1476	7	2 1 13
		2.1372	8	1 1 -18
		2.1306	6	2 0 17
		2.1009	3	2 2 0
13	2.0834(7)	2.0836	5	2 1 -14
		2.0803	2	2 2 -3
33	2.0117(4)	2.0164	9	1 3 1
		2.0103	14	3 1 2
		1.9863	7	3 1 -4
		1.9751	4	0 2 19
87	1.9637(2)	1.9689	16	3 1 5
		1.9597	30	1 2 -16
12	1.9214(7)	1.9245	11	3 1 -7
48	1.8999(3)	1.9039	10	2 0 20
		1.9003	10	1 2 17
		1.8983	4	3 1 8
		1.8982	9	1 1 21
11	1.8623(9)	1.8617	9	0 0 24
21	1.8389(6)	1.8395	13	3 1 -10
19	1.8022(16)	1.8076	9	1 3 -11
9	1.7846(6)	1.7874	11	1 2 -19
9	1.7339(13)	1.7405	5	1 3 13
		1.7350	1	3 0 18
		1.7299	1	0 4 8
16	1.7042(4)	1.7059	10	3 1 14
		1.7021	3	1 1 -24
18	1.6508(10)	1.6650	2	3 2 -2
		1.6605	2	0 4 11
		1.6549	4	0 0 27
		1.6513	2	2 3 -4
		1.6359	3	3 1 -16
		1.6339	2	1 2 -22
40	1.5976(12)	1.6042	3	0 2 25
		1.6009	9	3 1 17
		1.5997	2	2 3 8
		1.5996	2	0 3 21
44	1.5843(3)	1.5881	14	4 1 0
		1.5868	15	1 2 23
		1.5792	7	1 4 3
16	1.5467(14)	1.5532	6	1 4 6
		1.5397	3	1 1 -27
		1.5316	5	3 1 -19
21	1.5088(5)	1.5126	11	4 1 -9
		1.5018	3	2 3 -13
15	1.4594(3)	1.4614	2	0 2 28
		1.4608	9	4 1 12
		1.4433	2	0 5 4
12	1.4318(4)	1.4330	2	2 3 -16
		1.4317	6	1 3 22
17	1.4007(6)	1.4085	3	5 0 8
		1.4038	2	1 1 -30
		1.4014	2	1 4 15
		1.3997	3	1 3 -23
		1.3944	4	3 3 -3
35	1.3743(3)	1.3803	8	1 2 -28
		1.3765	5	3 3 -6
		1.3747	2	4 2 -1
		1.3727	2	2 4 -2
		1.3671	2	0 3 27
		1.3650	4	2 4 4
18	1.3389(2)	1.3480	3	3 3 9
		1.3445	3	2 4 7
		1.3381	2	3 1 -25
		1.3378	4	1 4 18
24	1.3047(3)	1.3145	2	2 4 10
		1.3109	3	3 3 12
		1.3085	3	1 3 -26
		1.3065	2	5 1 1
		1.3049	2	5 1 -2
		1.3036	3	2 0 32
		1.3027	3	4 2 11
		1.2982	2	5 1 4

Table 4. Data collection and structure refinement details for fuettererite.

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation	Mo$K\alpha$ (λ = 0.71075 Å)
Temperature	298(2) K
Structural Formula	$Pb_3Cu^{2+}{}_6Te^{6+}O_6(OH)_7Cl_5$
Space group	*R*-3
Unit cell dimensions	a = 8.4035(12) Å
	c = 44.681(4) Å
Z	6
Volume	2732.6(6) Å^3
Density (for above formula)	5.552 g cm^{-3}
Absorption coefficient	36.835 mm^{-1}
F(000)	4008
Crystal size	50 × 40 × 35 μm
θ range	3.34 to 25.02°
Index ranges	$-10 \le h \le 9$, $-10 \le k \le 10$, $-52 \le l \le 52$
Reflections collected/unique	7475/1074 [R_{int} = 0.086]
Reflections with $F_o > 4\sigma F$	971
Completeness to θ = 25.02°	99.2%
Max. and min. transmission	0.3588 and 0.2603
Refinement method	Full-matrix least-squares on F^2
Parameters refined	93
GoF	1.053
Final R indices [$F_o > 4\sigma F$]	R_1 = 0.0307, wR_2 = 0.0629
R indices (all data)	R_1 = 0.0350, wR_2 = 0.0649
Largest diff. peak/hole	+2.23/–1.43 e A^{-3}

Notes: $R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})|/\Sigma[F_o^2]$. GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where a is 0.0122, b is 42.3265 and P is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$.

Table 5. Fractional coordinates and atomic displacement parameters for fuettererite.

	x/*a*	*y*/*b*	*z*/*c*	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb	0.31093(5)	0.08441(5)	0.292530(8)	0.02421(16)	0.0252(3)	0.0258(3)	0.0215(2)	0.00081(14)	-0.00011(15)	0.01269(19)
Te	0.0000	0.0000	0.21811(2)	0.0151(2)	0.0156(4)	0.0156(4)	0.0142(5)	0.000	0.000	0.00781(18)
Cu1	0.29295(15)	0.87164(15)	0.21204(2)	0.0182(3)	0.0174(6)	0.0177(7)	0.0194(6)	0.0004(4)	-0.0015(4)	0.0087(5)
Cu2	0.42162(15)	0.29485(15)	0.21574(2)	0.0185(3)	0.0173(6)	0.0177(6)	0.0203(6)	-0.0004(4)	0.0004(4)	0.0087(5)
Cl1	0.3333	0.6667	0.1667	0.0238(13)	0.027(2)	0.027(2)	0.018(3)	0.000	0.000	0.0133(10)
Cl2	0.6667	0.3333	0.3333	0.0308(14)	0.036(2)	0.036(2)	0.020(3)	0.000	0.000	0.0181(12)
Cl3	0.6667	0.3333	0.25842(8)	0.0217(9)	0.0238(14)	0.0238(14)	0.0175(19)	0.000	0.000	0.0119(7)
Cl4	0.3307(4)	0.4253(3)	0.30055(5)	0.0282(6)	0.0279(14)	0.0250(14)	0.0293(13)	-0.0021(10)	-0.0002(10)	0.0113(11)
O1	0.0805(8)	0.8642(8)	0.19380(12)	0.0169(14)	0.026(4)	0.017(3)	0.014(3)	-0.003(2)	-0.001(2)	0.016(3)
O2	0.8640(9)	0.7773(8)	0.24186(12)	0.0192(14)	0.022(4)	0.026(4)	0.013(3)	0.002(3)	0.003(3)	0.014(3)
OH3	0.4826(8)	0.1181(9)	0.19776(13)	0.0195(15)	0.020(4)	0.025(4)	0.012(3)	0.000(3)	-0.001(3)	0.010(3)
H3	0.490(12)	0.107(12)	0.1781(6)	0.023						
OH4	0.3710(8)	0.4889(8)	0.23097(13)	0.0169(14)	0.017(3)	0.017(3)	0.016(3)	0.000(3)	-0.001(3)	0.007(3)
H4	0.361(12)	0.477(12)	0.2509(5)	0.020						
OH5	0.0000	0.0000	0.3046(2)	0.027(3)	0.031(4)	0.031(4)	0.019(6)	0.000	0.000	0.016(2)
H5	0.0000	0.0000	0.3247(5)	0.033						

Note: All sites were assigned full occupancy.

Table 6. Selected bond lengths (Å) in fuettererite.

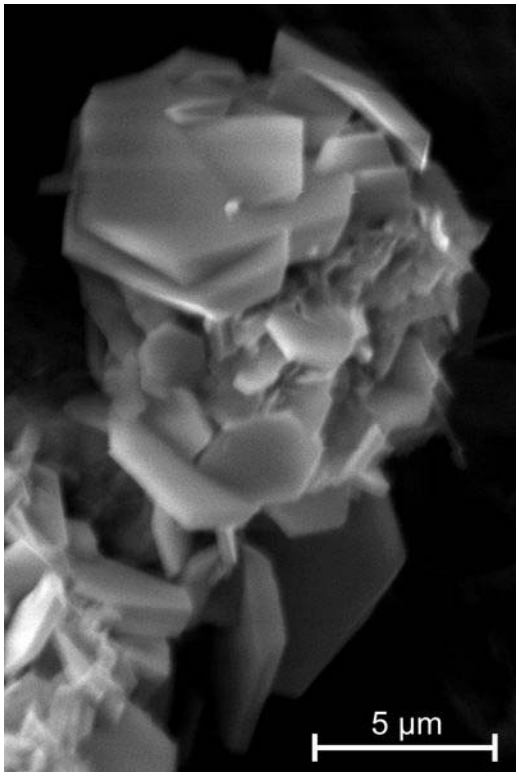
Pb–O2	2.385(5)	Cu1–O1	1.935(6)	Cu2–OH3	1.968(6)	
Pb–OH5	2.402(2)	Cu1–OH4	1.981(6)	Cu2–OH4	1.999(6)	
Pb–Cl4	2.808(2)	Cu1–OH3	1.984(7)	Cu2–OH3	2.003(6)	
Pb–Cl4	3.043(3)	Cu1–OH4	2.009(6)	Cu2–O2	2.071(6)	
Pb–Cl3	3.0630(18)	Cu1–O2	2.541(6)	Cu2–O1	2.362(6)	
Pb–Cl2	3.2222(5)	Cu1–Cl1	2.7888(11)	Cu2–Cl3	2.705(3)	
Pb–Cl4	3.262(3)	<Cu–φ>	2.207	<Cu–φ>	2.185	
Pb–Cl4	3.357(2)					
<Pb–φ>	2.943	Hydrogen bonding				

		D–H	d(D–H)	d(H…A)	<DHA	d(D…A)	A
Te–O1 (×3)	1.927(6)	OH3–H3	0.89(2)	1.75(3)	172(9)	2.634(8)	O1
Te–O2 (×3)	1.948(6)	OH4–H4	0.90(2)	2.25(2)	176(8)	3.144(6)	Cl4
<Te–O>	1.938	OH5–H5	0.90(2)	2.737(16)	132.5(4)	3.408(9)	Cl4 (×3)

Table 7. Bond valence sums for fuettererite. Values are expressed in valence units.

	Cl1	Cl2	Cl3	Cl4	O1	O2	OH3	OH4	OH5	Σ
Pb		0.154 ×6↓	0.237 ×3↓	0.472 0.250 0.138 0.107		0.423			0.408 ×3↓	2.189
Cu1	0.119 ×6↓				0.501	0.097	0.439	0.442 0.410		2.008
Cu2			0.149 ×3↓		0.158	0.347	0.458 0.417	0.421		1.950
Te					0.973 ×3→	0.920 ×3→				5.679
H3					0.205		0.795			1.000
H4				0.195				0.805		1.000
H5				0.075 ×3→					0.775	1.000
Σ	0.714	0.924	1.158	1.237	1.837	1.787	2.109	2.078	1.999	

Notes: All values are based upon full occupancies. Multiplicity is indicated by ×→↓. Pb^{2+}–O bond strengths from Krivovichev and Brown (2001); Pb^{2+}–Cl and Cu^{2+}–Cl bond strengths from Brese and O'Keeffe (1991); Te^{6+}–O and Cu^{2+}–O bond strengths from Brown and Altermatt (1985); hydrogen-bond strengths based on H···O and H···Cl bond lengths, also from Brown and Altermatt (1985). .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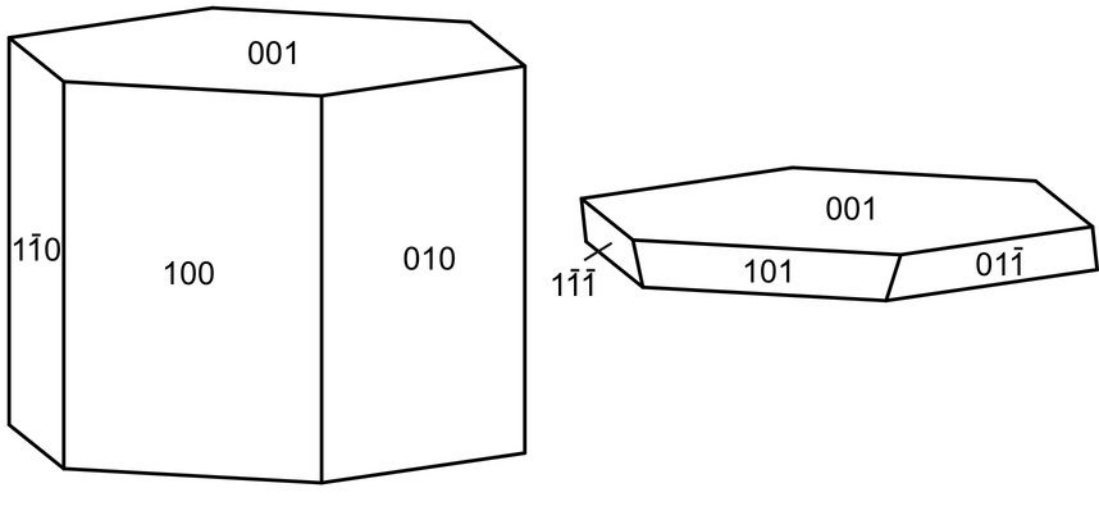
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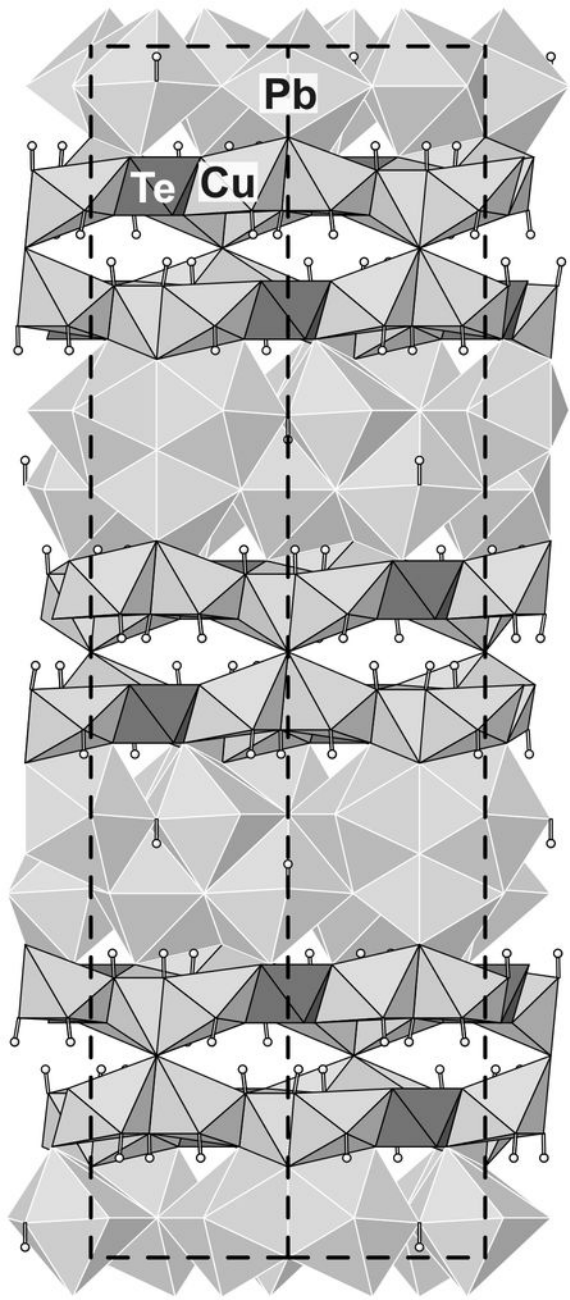
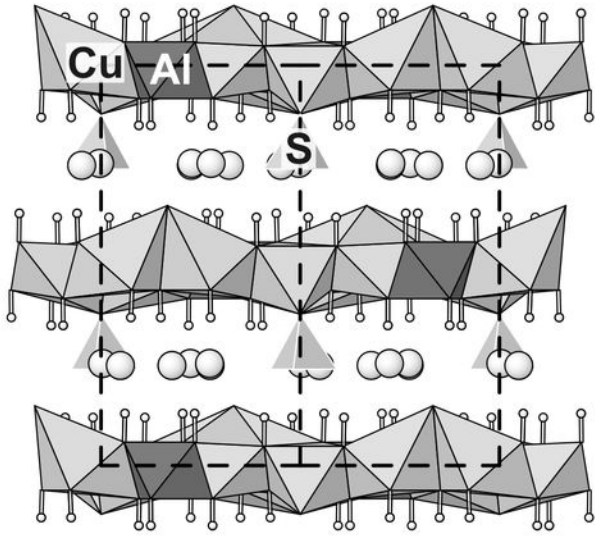


fuettererite



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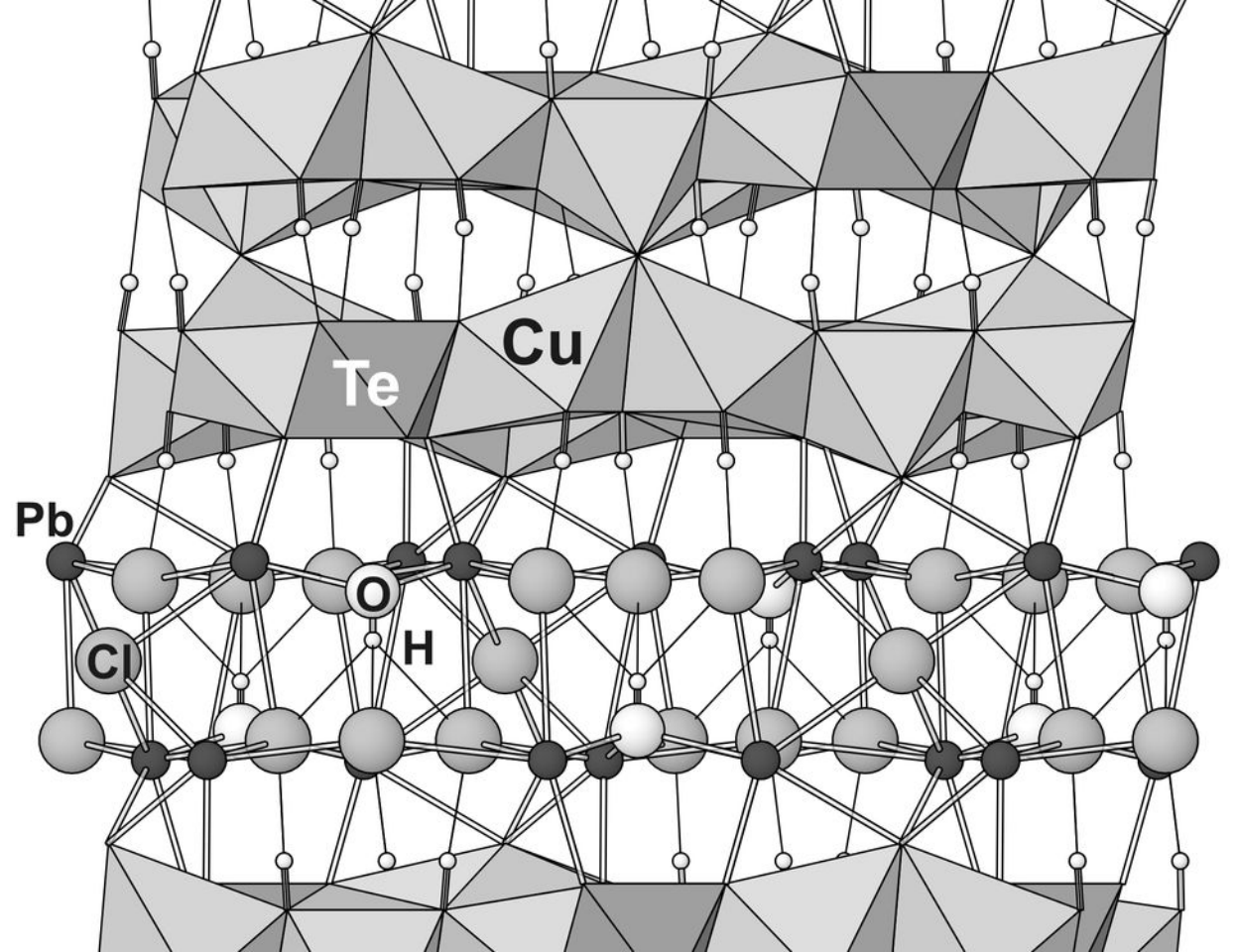
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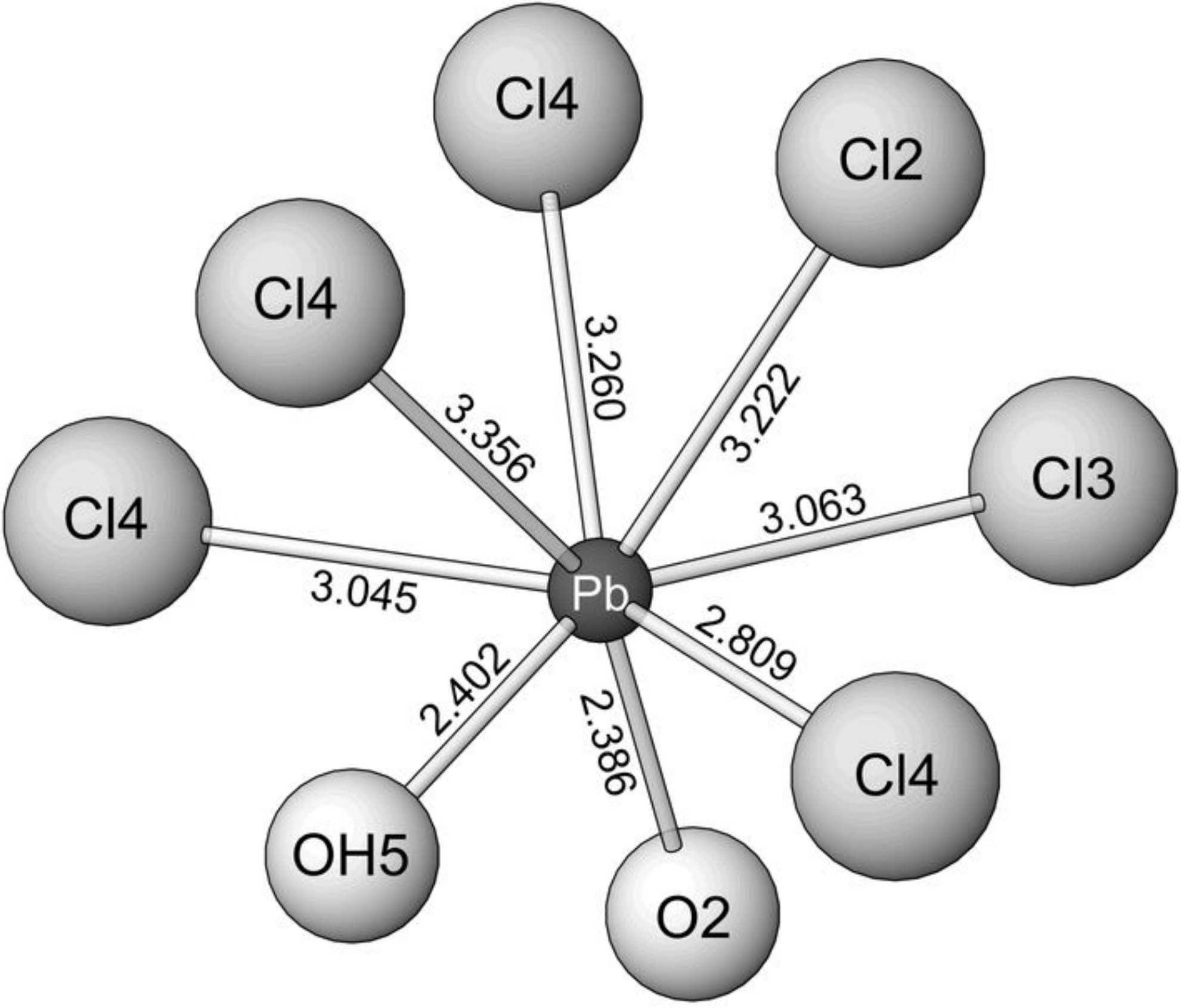
Cu
Pb
O
H
Cl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Cl4
Cl3
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Pb
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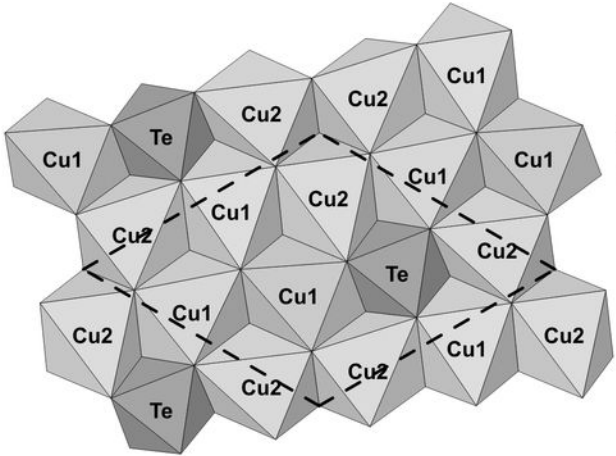
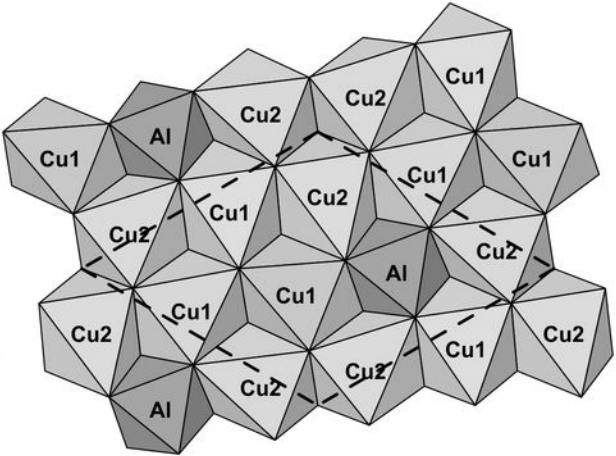
Cl4
OH5
O2



fuettererite



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