American Mineralogist, Volume 98, pages 506–511, 2013

Lead-tellurium oxysalts from Otto Mountain near Baker, California: VIII. Fuettererite, $Pb_3Cu_6^{2+}Te^{6+}O_6(OH)_7Cl_5$, a new mineral with double spangolite-type sheets

Anthony R. Kampf,[1,*] Stuart J. Mills,[2] Robert M. Housley,[3] and Joseph Marty[4]

[1]Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, California 90007, U.S.A.
[2]Geosciences, Museum Victoria, GPO Box 666, Melbourne 3001, Victoria, Australia
[3]Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, California 91125, U.S.A.
[4]5199 E. Silver Oak Road, Salt Lake City, Utah 84108, U.S.A.

Abstract

Fuettererite, $Pb_3Cu_6^{2+}Te^{6+}O_6(OH)_7Cl_5$, 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, with space group $R\overline{3}$, 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 ω = 2.04 and ε = 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 apfu) is: $Pb_{2.88}Cu_{5.92}^{2+}Al_{0.07}Te_{1.13}^{6+}O_{6.59}(OH)_{6.12}Cl_{5.29}$. 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$\overline{1}$) 53, 2.6686 (12$\overline{4}$) 49, 2.5289 (12$\overline{7}$) 41, 2.2772 (1.2.11) 38, 1.9637 (315, 1.2.$\overline{16}$) 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. 2013, this issue), 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

* E-mail: akampf@nhm.org

0003-004X/13/0203–506$05.00/DOI: http://dx.doi.org/10.2138/am.2013.4218

TABLE 1. New minerals described from Otto Mountain

Mineral	Ideal Formula	Reference
Ottoite	$Pb_2Te^{6+}O_5$	Kampf et al. (2010a)
Housleyite	$Pb_6Cu^{2+}Te_4^{6+}O_{18}(OH)_2$	Kampf et al. (2010b)
Thorneite	$Pb_6(Te_2^{6+}O_{10})(CO_3)Cl_2(H_2O)$	Kampf et al. (2010c)
Markcooperite	$Pb_2(UO_2)Te^{6+}O_6$	Kampf et al. (2010d)
Timroseite	$Pb_2Cu_5^{2+}(Te^{6+}O_6)_2(OH)_2$	Kampf et al. (2010e)
Paratimroseite	$Pb_2Cu_4^{2+}(Te^{6+}O_6)_2(H_2O)_2$	Kampf et al. (2010e)
Telluroperite	$Pb_3Te^{4+}O_4Cl_2$	Kampf et al. (2010f)
Chromschieffelinite	$Pb_{10}Te_6^{6+}O_{20}(CrO_4)(H_2O)_5$	Kampf et al. (2012)
Fuettererite	$Pb_3Cu_6^{2+}Te^{6+}O_6(OH)_7Cl_5$	This study
Agaite	$Pb_3Cu^{2+}Te^{6+}O_5(OH)_2(CO_3)$	Kampf et al. (2013)

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 co-type specimen are deposited in the Natural History Museum of Los Angeles County, catalog 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 co-type 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 (R.M.H. and J.M.). 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 co-type 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 acanthite, agaite, boleite, brochantite, burckhardtite, calcite, caledonite, celestine, cerussite, chromschieffelinite, chrysocolla, creaseyite, devilline, diaboleite, eztlite, fluorite, fornacite, frankhawthorneite, gold, gypsum, hemimorphite, hessite, housleyite, jarosite, khinite, kuranakhite, leadhillite, linarite, malachite, markcooperite, mattheadleyite, mcalpineite, mimetite, mottramite, munakataite, murdochite, ottoite, paratimroseite, perite, plumbojarosite, plumbotsumite, pyrite, sonoraite, sphalerite, thorneite, vanadinite, vauquelinite, and xocomacatlite.

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 co-type 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

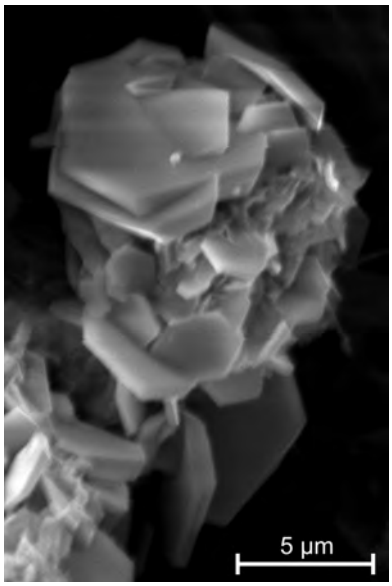

FIGURE 1. SEM image of fuettererite tablets on the co-type specimen.

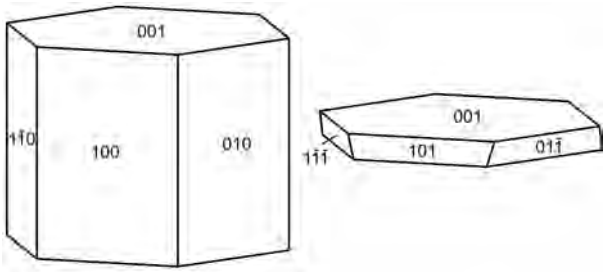

FIGURE 2. Crystal drawings (clinographic projections) of fuettererite showing prismatic (**left**) and tabular (**right**) habits.

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, 2010b, 2010c, 2010d, 2010e, 2012, 2013; Mills et al. 2009, 2010).

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

The empirical formula (based on 18 O + Cl apfu) 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$K\alpha$ radiation. Observed powder *d*-values (with standard deviations) and intensities were derived by profile fitting using JADE 9.3 software.

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 $\overline{3}$
100	3.733(5)	3.7234	100	0 0 12
27	3.697(5)	3.6594	30	1 1 $\overline{6}$
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 $\overline{12}$
53	2.749(5)	2.7455	40	1 2 $\overline{1}$
10	2.729(2)	2.7301	8	2 1 $\overline{2}$
49	2.6686(7)	2.6709	39	1 2 $\overline{4}$
26	2.6275(10)	2.6290	26	1 2 5
41	2.5289(15)	2.5261	48	1 2 $\overline{7}$
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 $\overline{15}$
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 $\overline{18}$
		2.1306	6	2 0 17
		2.1009	3	2 2 0
13	2.0834(7)	2.0836	5	2 1 $\overline{14}$
		2.0803	2	2 2 $\overline{3}$
33	2.0117(4)	2.0164	9	1 3 1
		2.0103	14	3 1 2
		1.9863	7	3 1 $\overline{4}$
		1.9751	4	0 2 19
87	1.9637(2)	1.9689	16	3 1 5
		1.9597	30	1 2 $\overline{16}$
12	1.9214(7)	1.9245	11	3 1 $\overline{7}$
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 $\overline{10}$
19	1.8022(16)	1.8076	9	1 3 $\overline{11}$
9	1.7846(6)	1.7874	11	1 2 $\overline{19}$
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 $\overline{24}$
18	1.6508(10)	1.6650	2	3 2 $\overline{2}$
		1.6605	2	0 4 11
		1.6549	4	0 0 27
		1.6513	2	2 3 $\overline{4}$
		1.6359	3	3 1 $\overline{16}$
		1.6339	2	1 2 $\overline{22}$
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 $\overline{27}$
		1.5316	5	3 1 $\overline{19}$
21	1.5088(5)	1.5126	11	4 1 $\overline{9}$
		1.5018	3	2 3 $\overline{13}$
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 $\overline{16}$
		1.4317	6	1 3 22
		1.4085	3	5 0 8
		1.4038	2	1 1 $\overline{30}$
17	1.4007(6)	1.4014	2	1 4 15
		1.3997	3	1 3 $\overline{23}$
		1.3944	4	3 3 $\overline{3}$
35	1.3743(3)	1.3803	8	1 2 $\overline{28}$
		1.3765	5	3 3 $\overline{6}$
		1.3747	2	4 2 $\overline{1}$
		1.3727	2	2 4 $\overline{2}$
		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 $\overline{25}$
		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 $\overline{26}$
		1.3065	2	5 1 1
		1.3049	2	5 1 $\overline{2}$
		1.3036	3	2 0 32
		1.3027	3	4 2 11
		1.2982	2	5 1 4

Data (in angstroms) 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 are attributable to the use of Mo$K\alpha$ 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 the H atoms 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

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	$Pb_3Cu_6^{2+}Te^{6+}O_6(OH)_7Cl_5$
Space group	$R\bar{3}$
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 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 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 7. Bond valence sums for fuettererite

	Cl1	Cl2	Cl3	Cl4	O1	O2	OH3	OH4	OH5	Σ
Pb		0.154 × 6↓	0.237 × 3↓	0.472		0.423			0.408 ×3↓	2.189
				0.250						
				0.138						
				0.107						
Cu1	0.119 ×6↓				0.501	0.097	0.439	0.442		2.008
								0.410		
Cu2			0.149 ×3↓		0.158	0.347	0.458	0.421		1.950
							0.417			
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: Values are expressed in valence units. 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).

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. (CIF and data set deposited online[1].)

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, $Cu_6Al(SO_4)(OH)_{12}Cl{\cdot}3H_2O$ (Hawthorne et al. 1993), except that in spangolite it is composed of CuO_5Cl, CuO_6,

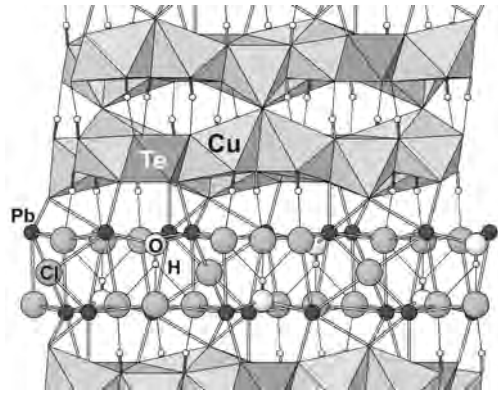

Figure 4. Detail of layers in fuettererite structure with Pb coordination shown in "ball-and-stick" style. Hydrogen bonds are shown as single black lines.

[1] Deposit item AM-13-017, Data set and CIF. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

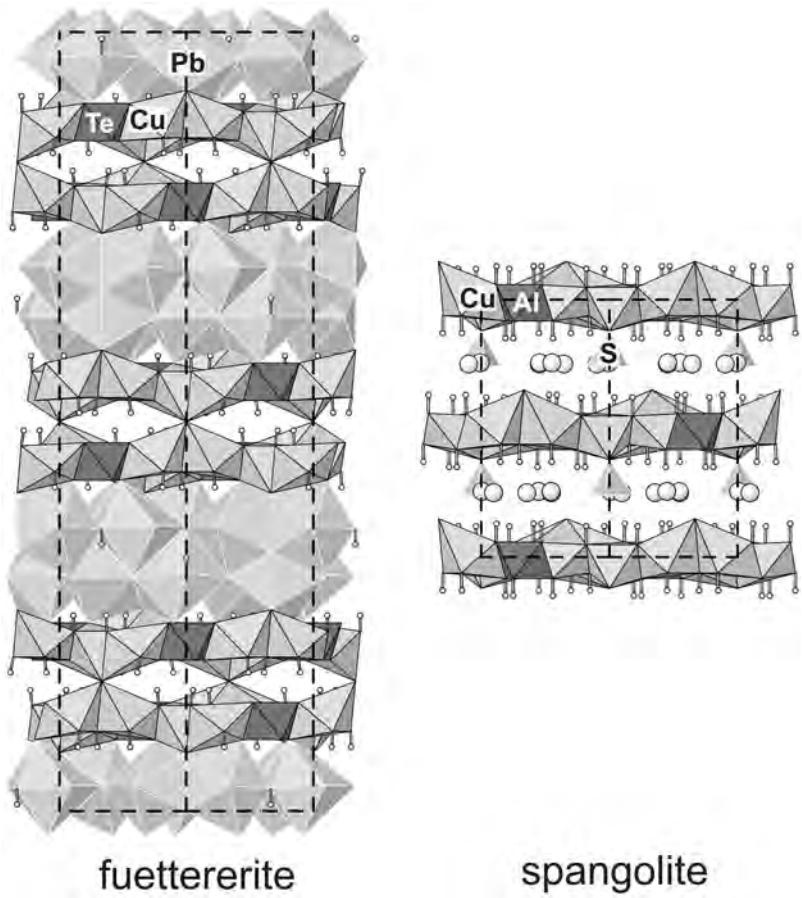

Figure 3. Structures of fuettererite and spangolite viewed down [110] with **c** vertical. Unit cells are shown as dashed lines.

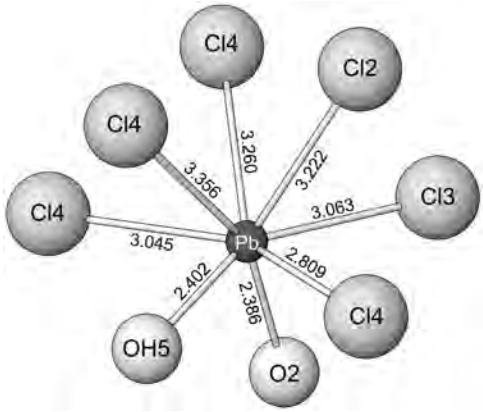

FIGURE 5. Pb coordination in fuettererite. The lopsided distributions of bond lengths are attributable to the localization of the lone-pair electrons. Bond lengths are given in angstroms.

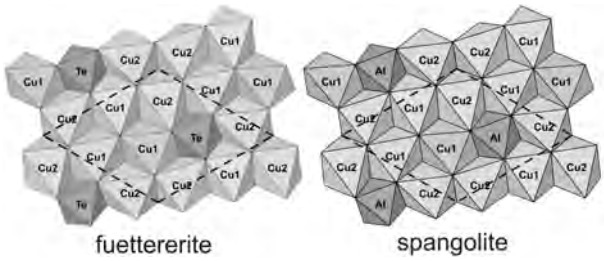

FIGURE 6. Octahedral sheets in the structures of fuettererite and spangolite, in both cases viewed down **c**.

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).

ACKNOWLEDGMENTS

The paper benefited from comments by reviewers Chi Ma and John M. Hughes. Jerry Baird is thanked for providing the co-type specimen of fuettererite. The Caltech EMP analyses were supported by a grant from the Northern California Mineralogical Association. The remainder of this study was funded by the John Jago Trelawney Endowment to the Mineral Sciences Department of the Natural History Museum of Los Angeles County.

REFERENCES CITED

Burla, M.C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G.L., De Caro, L., Giacovazzo, C., Polidori, G., and Spagna, R. (2005) SIR2004: An improved tool for crystal structure determination and refinement. Journal of Applied Crystallography, 38, 381–388.

Brese, N.E. and O'Keeffe, M. (1991) Bond-valence parameters for solids. Acta Crystallographica, B47, 192–197.

Brown, I.D. and Altermatt, D. (1985) Bond-valence parameters from a systematic analysis of the inorganic crystal structure database. Acta Crystallographica, B41, 244–247.

Hawthorne, F.C., Kimata, M., and Eby, R.K. (1993) The crystal structure of spangolite, a complex copper sulfate sheet mineral. American Mineralogist, 78, 649–652.

Higashi, T. (2001) ABSCOR. Rigaku Corporation, Tokyo, Japan.

Housley, R.M., Kampf, A.R., Mills, S.J., Marty, J., and Thorne, B. (2011) The remarkable occurrence of rare secondary tellurium minerals at Otto Mountain near Baker, California – including seven new species. Rocks and Minerals, 86, 132–142.

Kampf, A.R., Housley, R.M., Mills, S.J., Marty, J., and Thorne, B. (2010a) Lead-tellurium oxysalts from Otto Mountain near Baker, California: I. Ottoite, Pb_2TeO_5, a new mineral with chains of tellurate octahedra. American Mineralogist, 95, 1329–1336.

Kampf, A.R., Marty, J., and Thorne, B. (2010b) Lead-tellurium oxysalts from Otto Mountain near Baker, California: II. Housleyite, $Pb_6CuTe_4TeO_{18}(OH)_2$, a new mineral with Cu-Te octahedral sheets. American Mineralogist, 95, 1337–1342.

Kampf, A.R., Housley, R.M., and Marty, J. (2010c) Lead-tellurium oxysalts from Otto Mountain near Baker, California: III. Thorneite, $Pb_6(Te_2O_{10})(CO_3)Cl_2(H_2O)$, the first mineral with edge-sharing octahedral dimers. American Mineralogist, 95, 1548–1553.

Kampf, A.R., Mills, S.J., Housley, R.M., Marty, J., and Thorne, B. (2010d) Lead-tellurium oxysalts from Otto Mountain near Baker, California: IV. Markcooperite, $Pb_2(UO_2)TeO_6$, the first natural uranyl tellurate. American Mineralogist, 95, 1554–1559.

——— (2010e) Lead-tellurium oxysalts from Otto Mountain near Baker, California: V. Timroseite, $Pb_2Cu^{2+}_5(Te^{6+}O_6)_2(OH)_2$, and paratimroseite, $Pb_2Cu^{2+}_4(Te^{6+}O_6)_2(H_2O)_2$, new minerals with edge-sharing Cu-Te octahedral chains. American Mineralogist, 95, 1560–1568.

——— (2010f) Lead–tellurium oxysalts from Otto Mountain near Baker, California: VI. Telluroperite, $Pb_3Te^{4+}O_4Cl_2$, the Te analogue of perite and nadorite. American Mineralogist, 95, 1569–1573.

Kampf, A.R., Mills, S.J., and Housley, R.M. (2010g) The crystal structure of munakataite, $Pb_2Cu_2(Se^{4+}O_3)(SO_4)(OH)_4$, from Otto Mountain, San Bernardino County, California, USA. Mineralogical Magazine, 74, 991–998.

Kampf, A.R., Mills, S.J., Housley, R.M., Rumsey, M.S., and Spratt, J. (2012) Lead-tellurium oxysalts from Otto Mountain near Baker, California: VII. Chromschieffelinite, $Pb_{10}Te_6O_{20}(CrO_4)(H_2O)_5$, the chromate analogue of schieffelinite. American Mineralogist, 97, 212–219.

Kampf, A.R., Mills, S.J., Housley, R.M., and Marty, J. (2013) Lead-tellurium oxysalts from Otto Mountain near Baker, California: IX. Agaite, $Pb_3Cu^{2+}Te^{6+}O_5(OH)_2(CO_3)$, a new mineral with CuO_5-TeO_6 polyhedral sheets. American Mineralogist, 98, 512–517.

Krivovichev, S.V. and Brown, I.D. (2001) Are the compressive effects of encapsulation an artifact of the bond valence parameters? Zeitschrift für Kristallographie, 216, 245–247.

Mills, S.J., Kampf, A.R., Kolitsch, U., Housley, R.M., and Raudsepp, M. (2010) The crystal chemistry and crystal structure of kuksite, $Pb_3Zn_3Te^{6+}P_2O_{14}$, and a note on the crystal structure of yafsoanite, $(Ca,Pb)_3Zn(TeO_6)_2$. American Mineralogist, 95, 933–938.

Mills, S.J., Kolitsch, U., Miyawaki, R., Groat, L.A., and Poirier, G. (2009) Joëlbruggerite, $Pb_3Zn_3(Sb^{5+},Te^{6+})As_2O_{13}(OH,O)$, the Sb^{5+} analogue of dugganite, from the Black Pine mine, Montana. American Mineralogist, 94, 1012–1017.

Sheldrick, G.M. (2008) A short history of *SHELX*. Acta Crystallographica, A64, 112–122.

MANUSCRIPT RECEIVED MAY 7, 2012
MANUSCRIPT ACCEPTED OCTOBER 14, 2012
MANUSCRIPT HANDLED BY ANDREW MCDONALD

```
data_otto13

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'H7 Cl5 Cu6 O13 Pb3 Te'
_chemical_formula_weight          1522.72

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'Pb'  'Pb'  -3.3944  10.1111
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Te'  'Te'  -0.5308   1.6751
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cu'  'Cu'   0.3201   1.2651
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl'  'Cl'   0.1484   0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            ?
_symmetry_space_group_name_H-M    R-3

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-y, x-y, z'
 '-x+y, -x, z'
 'x+2/3, y+1/3, z+1/3'
 '-y+2/3, x-y+1/3, z+1/3'
 '-x+y+2/3, -x+1/3, z+1/3'
 'x+1/3, y+2/3, z+2/3'
 '-y+1/3, x-y+2/3, z+2/3'
 '-x+y+1/3, -x+2/3, z+2/3'
 '-x, -y, -z'
 'y, -x+y, -z'
 'x-y, x, -z'
 '-x+2/3, -y+1/3, -z+1/3'
 'y+2/3, -x+y+1/3, -z+1/3'
 'x-y+2/3, x+1/3, -z+1/3'
 '-x+1/3, -y+2/3, -z+2/3'
```

```
 'y+1/3, -x+y+2/3, -z+2/3'
 'x-y+1/3, x+2/3, -z+2/3'

_cell_length_a                    8.4035(12)
_cell_length_b                    8.4035(12)
_cell_length_c                    44.681(4)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                 120.00
_cell_volume                      2732.6(6)
_cell_formula_units_Z             6
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     ?
_cell_measurement_theta_min       ?
_cell_measurement_theta_max       ?

_exptl_crystal_description        ?
_exptl_crystal_colour             ?
_exptl_crystal_size_max           0.05
_exptl_crystal_size_mid           0.04
_exptl_crystal_size_min           0.04
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     5.552
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              4008
_exptl_absorpt_coefficient_mu     36.835
_exptl_absorpt_correction_type    ?
_exptl_absorpt_correction_T_min   0.2603
_exptl_absorpt_correction_T_max   0.3588
_exptl_absorpt_process_details    ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71075
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             7475
_diffrn_reflns_av_R_equivalents   0.0864
_diffrn_reflns_av_sigmaI/netI     0.0587
_diffrn_reflns_limit_h_min        -10
_diffrn_reflns_limit_h_max        9
_diffrn_reflns_limit_k_min        -10
_diffrn_reflns_limit_k_max        10
```

```
_diffrn_reflns_limit_l_min        -52
_diffrn_reflns_limit_l_max        52
_diffrn_reflns_theta_min          3.34
_diffrn_reflns_theta_max          25.02
_reflns_number_total              1074
_reflns_number_gt                 971
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        ?
_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0122P)^2^+42.3265P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          1074
_refine_ls_number_parameters      93
_refine_ls_number_restraints      3
_refine_ls_R_factor_all           0.0350
_refine_ls_R_factor_gt            0.0307
_refine_ls_wR_factor_ref          0.0649
_refine_ls_wR_factor_gt           0.0629
_refine_ls_goodness_of_fit_ref    1.053
_refine_ls_restrained_S_all       1.051
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
```

```
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Pb Pb 0.31093(5) 0.08441(5) 0.292530(8) 0.02421(16) Uani 1 1 d . . .
Te Te 0.0000 0.0000 0.21811(2) 0.0151(2) Uani 1 3 d S . .
Cu1 Cu 0.29295(15) 0.87164(15) 0.21204(2) 0.0182(3) Uani 1 1 d . . .
Cu2 Cu 0.42162(15) 0.29485(15) 0.21574(2) 0.0185(3) Uani 1 1 d . . .
Cl1 Cl 0.3333 0.6667 0.1667 0.0238(13) Uani 1 6 d S . .
Cl2 Cl 0.6667 0.3333 0.3333 0.0308(14) Uani 1 6 d S . .
Cl3 Cl 0.6667 0.3333 0.25842(8) 0.0217(9) Uani 1 3 d S . .
Cl4 Cl 0.3307(4) 0.4253(3) 0.30055(5) 0.0282(6) Uani 1 1 d . . .
O1 O 0.0805(8) 0.8642(8) 0.19380(12) 0.0169(14) Uani 1 1 d . . .
O2 O 0.8640(9) 0.7773(8) 0.24186(12) 0.0192(14) Uani 1 1 d . . .
OH3 O 0.4826(8) 0.1181(9) 0.19776(13) 0.0195(15) Uani 1 1 d D . .
H3 H 0.490(12) 0.107(12) 0.1781(6) 0.023 Uiso 1 1 d D . .
OH4 O 0.3710(8) 0.4889(8) 0.23097(13) 0.0169(14) Uani 1 1 d D . .
H4 H 0.361(12) 0.477(12) 0.2509(5) 0.020 Uiso 1 1 d D . .
OH5 O 0.0000 0.0000 0.3046(2) 0.027(3) Uani 1 3 d SD . .
H5 H 0.0000 0.0000 0.3247(5) 0.033 Uiso 1 3 d SD . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Pb 0.0252(3) 0.0258(3) 0.0215(2) 0.00081(14) -0.00011(15) 0.01269(19)
Te 0.0156(4) 0.0156(4) 0.0142(5) 0.000 0.000 0.00781(18)
Cu1 0.0174(6) 0.0177(7) 0.0194(6) 0.0004(4) -0.0015(4) 0.0087(5)
Cu2 0.0173(6) 0.0177(6) 0.0203(6) -0.0004(4) 0.0004(4) 0.0087(5)
Cl1 0.027(2) 0.027(2) 0.018(3) 0.000 0.000 0.0133(10)
Cl2 0.036(2) 0.036(2) 0.020(3) 0.000 0.000 0.0181(12)
Cl3 0.0238(14) 0.0238(14) 0.0175(19) 0.000 0.000 0.0119(7)
Cl4 0.0279(14) 0.0250(14) 0.0293(13) -0.0021(10) -0.0002(10) 0.0113(11)
O1 0.026(4) 0.017(3) 0.014(3) -0.003(2) -0.001(2) 0.016(3)
O2 0.022(4) 0.026(4) 0.013(3) 0.002(3) 0.003(3) 0.014(3)
OH3 0.020(4) 0.025(4) 0.012(3) 0.000(3) -0.001(3) 0.010(3)
OH4 0.017(3) 0.017(3) 0.016(3) 0.000(3) -0.001(3) 0.007(3)
OH5 0.031(4) 0.031(4) 0.019(6) 0.000 0.000 0.016(2)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
```

```
 treatment of cell esds is used for estimating esds involving l.s. planes.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
Pb O2 2.385(5) 2_655 ?
Pb OH5 2.402(2) . ?
Pb Cl4 2.808(2) . ?
Pb Cl4 3.043(3) 3 ?
Pb Cl3 3.0630(18) . ?
Pb Cl2 3.2222(5) . ?
Pb Cl4 3.262(3) 2_655 ?
Pb Cl4 3.357(2) 18_545 ?
Pb OH4 4.018(6) 2_655 ?
Pb O2 4.025(6) 1_445 ?
Te O1 1.927(6) 3_455 ?
Te O1 1.927(6) 1_545 ?
Te O1 1.927(6) 2_665 ?
Te O2 1.948(6) 2_655 ?
Te O2 1.948(6) 3_565 ?
Te O2 1.948(6) 1_445 ?
Cu1 O1 1.935(6) . ?
Cu1 OH4 1.981(6) 2_665 ?
Cu1 OH3 1.984(7) 1_565 ?
Cu1 OH4 2.009(6) 3_565 ?
Cu1 O2 2.541(6) 2_665 ?
Cu1 Cl1 2.7888(11) . ?
Cu2 OH3 1.968(6) . ?
Cu2 OH4 1.999(6) . ?
Cu2 OH3 2.003(6) 3_665 ?
Cu2 O2 2.071(6) 2_655 ?
Cu2 O1 2.362(6) 2_665 ?
Cu2 Cl3 2.705(3) . ?
Cl1 Cu1 2.7886(11) 13_565 ?
Cl1 Cu1 2.7887(11) 14_455 ?
Cl1 Cu1 2.7887(11) 15 ?
Cl1 Cu1 2.7889(11) 3_565 ?
Cl1 Cu1 2.7889(11) 2_665 ?
Cl1 Cu2 4.1760(12) 15 ?
Cl1 Cu2 4.1760(12) 14_455 ?
Cl1 Cu2 4.1760(12) 2_665 ?
Cl1 Cu2 4.1760(12) 3_565 ?
Cl1 Cu2 4.1760(12) 13_565 ?
Cl2 Pb 3.2221(5) 17 ?
Cl2 Pb 3.2221(5) 16_655 ?
Cl2 Pb 3.2221(5) 18_545 ?
Cl2 Pb 3.2222(5) 2_655 ?
Cl2 Pb 3.2222(5) 3_665 ?
Cl3 Cu2 2.705(3) 2_655 ?
Cl3 Cu2 2.705(3) 3_665 ?
Cl3 Pb 3.0629(18) 2_655 ?
```

```
Cl3 Pb 3.0629(18) 3_665 ?
Cl3 Cu1 4.126(2) 1_545 ?
Cl3 Cu1 4.126(2) 2_765 ?
Cl3 Cu1 4.126(2) 3_565 ?
Cl4 Pb 3.043(3) 2 ?
Cl4 Pb 3.262(3) 3_665 ?
Cl4 Pb 3.357(2) 17 ?
Cl4 Cu1 4.298(3) 2_665 ?
O1 Te 1.927(6) 1_565 ?
O1 Cu2 2.362(6) 3_565 ?
O1 Cu2 3.450(6) 1_565 ?
O1 Cu2 3.692(6) 13_565 ?
O1 Cu1 3.824(6) 3_465 ?
O1 Cu1 3.824(6) 15 ?
O1 Cu2 4.005(6) 15_455 ?
O1 Cu1 4.022(6) 2_665 ?
O2 Te 1.948(6) 1_665 ?
O2 Cu2 2.071(6) 3_665 ?
O2 Pb 2.385(5) 3_665 ?
O2 Cu1 2.541(6) 3_565 ?
O2 Cu1 3.541(6) 1_655 ?
O2 Cu2 3.962(6) 2_665 ?
O2 Pb 4.025(6) 1_665 ?
OH3 Cu1 1.984(6) 1_545 ?
OH3 Cu2 2.003(6) 2_655 ?
OH3 Cu2 3.699(6) 3_665 ?
OH3 Cu1 3.963(6) 14_445 ?
OH3 Cu1 3.973(6) 3 ?
OH3 Cu2 3.991(6) 13 ?
OH4 Cu1 1.981(6) 3_565 ?
OH4 Cu1 2.009(6) 2_665 ?
OH4 Cu2 3.958(6) 3_665 ?
OH4 Pb 4.018(6) 3_665 ?
OH5 Pb 2.402(2) 3 ?
OH5 Pb 2.402(2) 2 ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O2 Pb OH5 85.4(3) 2_655 . ?
O2 Pb Cl4 88.44(15) 2_655 . ?
OH5 Pb Cl4 76.90(6) . . ?
O2 Pb Cl4 96.39(15) 2_655 3 ?
OH5 Pb Cl4 72.35(5) . 3 ?
Cl4 Pb Cl4 148.33(8) . 3 ?
O2 Pb Cl3 73.94(15) 2_655 . ?
OH5 Pb Cl3 149.30(15) . . ?
Cl4 Pb Cl3 80.04(5) . . ?
Cl4 Pb Cl3 131.39(5) 3 . ?
O2 Pb Cl2 136.29(14) 2_655 . ?
```

OH5 Pb Cl2 125.7(2) . . ?
Cl4 Pb Cl2 72.72(5) . . ?
Cl4 Pb Cl2 120.40(4) 3 . ?
Cl3 Pb Cl2 64.30(6) . . ?
O2 Pb Cl4 113.19(16) 2_655 2_655 ?
OH5 Pb Cl4 136.78(11) . 2_655 ?
Cl4 Pb Cl4 138.51(8) . 2_655 ?
Cl4 Pb Cl4 67.21(9) 3 2_655 ?
Cl3 Pb Cl4 73.35(5) . 2_655 ?
Cl2 Pb Cl4 67.25(4) . 2_655 ?
O2 Pb Cl4 155.27(15) 2_655 18_545 ?
OH5 Pb Cl4 70.3(2) . 18_545 ?
Cl4 Pb Cl4 90.53(5) . 18_545 ?
Cl4 Pb Cl4 72.28(7) 3 18_545 ?
Cl3 Pb Cl4 130.12(7) . 18_545 ?
Cl2 Pb Cl4 66.12(4) . 18_545 ?
Cl4 Pb Cl4 83.24(5) 2_655 18_545 ?
O2 Pb Cu2 30.04(14) 2_655 . ?
OH5 Pb Cu2 108.7(2) . . ?
Cl4 Pb Cu2 76.23(5) . . ?
Cl4 Pb Cu2 120.83(5) 3 . ?
Cl3 Pb Cu2 45.32(6) . . ?
Cl2 Pb Cu2 106.27(2) . . ?
Cl4 Pb Cu2 104.60(4) 2_655 . ?
Cl4 Pb Cu2 166.43(5) 18_545 . ?
O2 Pb Cu1 37.35(15) 2_655 1_545 ?
OH5 Pb Cu1 106.2(2) . 1_545 ?
Cl4 Pb Cu1 122.85(5) . 1_545 ?
Cl4 Pb Cu1 74.04(5) 3 1_545 ?
Cl3 Pb Cu1 70.28(5) . 1_545 ?
Cl2 Pb Cu1 128.07(2) . 1_545 ?
Cl4 Pb Cu1 76.96(5) 2_655 1_545 ?
Cl4 Pb Cu1 145.48(5) 18_545 1_545 ?
Cu2 Pb Cu1 48.10(2) . 1_545 ?
O2 Pb OH4 63.35(17) 2_655 2_655 ?
OH5 Pb OH4 130.8(2) . 2_655 ?
Cl4 Pb OH4 134.04(10) . 2_655 ?
Cl4 Pb OH4 74.47(10) 3 2_655 ?
Cl3 Pb OH4 58.41(9) . 2_655 ?
Cl2 Pb OH4 102.31(9) . 2_655 ?
Cl4 Pb OH4 49.86(9) 2_655 2_655 ?
Cl4 Pb OH4 130.28(9) 18_545 2_655 ?
Cu2 Pb OH4 61.09(9) . 2_655 ?
Cu1 Pb OH4 28.65(8) 1_545 2_655 ?
O2 Pb O2 43.72(19) 2_655 1_445 ?
OH5 Pb O2 53.8(2) . 1_445 ?
Cl4 Pb O2 106.64(10) . 1_445 ?
Cl4 Pb O2 60.00(9) 3 1_445 ?
Cl3 Pb O2 115.93(10) . 1_445 ?
Cl2 Pb O2 179.31(9) . 1_445 ?
Cl4 Pb O2 113.42(10) 2_655 1_445 ?
Cl4 Pb O2 113.72(9) 18_545 1_445 ?
Cu2 Pb O2 73.75(8) . 1_445 ?
Cu1 Pb O2 52.47(8) 1_545 1_445 ?
OH4 Pb O2 78.31(12) 2_655 1_445 ?

```
O2 Pb Pb 72.16(15) 2_655 2 ?
OH5 Pb Pb 32.46(9) . 2 ?
Cl4 Pb Pb 48.60(5) . 2 ?
Cl4 Pb Pb 103.29(5) 3 2 ?
Cl3 Pb Pb 117.56(2) . 2 ?
Cl2 Pb Pb 116.088(13) . 2 ?
Cl4 Pb Pb 169.10(4) 2_655 2 ?
Cl4 Pb Pb 88.78(4) 18_545 2 ?
Cu2 Pb Pb 84.712(18) . 2 ?
Cu1 Pb Pb 106.222(17) 1_545 2 ?
OH4 Pb Pb 134.65(8) 2_655 2 ?
O2 Pb Pb 63.23(8) 1_445 2 ?
O2 Pb Pb 77.48(14) 2_655 3 ?
OH5 Pb Pb 32.46(9) . 3 ?
Cl4 Pb Pb 108.03(5) . 3 ?
Cl4 Pb Pb 43.80(5) 3 3 ?
Cl3 Pb Pb 150.08(6) . 3 ?
Cl2 Pb Pb 145.480(8) . 3 ?
Cl4 Pb Pb 110.96(5) 2_655 3 ?
Cl4 Pb Pb 79.37(4) 18_545 3 ?
Cu2 Pb Pb 107.331(18) . 3 ?
Cu1 Pb Pb 81.692(18) 1_545 3 ?
OH4 Pb Pb 100.60(9) 2_655 3 ?
O2 Pb Pb 34.35(8) 1_445 3 ?
Pb Pb Pb 60.0 2 3 ?
O2 Pb Te 18.21(15) 2_655 . ?
OH5 Pb Te 67.9(2) . . ?
Cl4 Pb Te 89.28(5) . . ?
Cl4 Pb Te 86.15(4) 3 . ?
Cl3 Pb Te 92.00(6) . . ?
Cl2 Pb Te 151.958(12) . . ?
Cl4 Pb Te 122.35(4) 2_655 . ?
Cl4 Pb Te 137.10(4) 18_545 . ?
Cu2 Pb Te 47.29(2) . . ?
Cu1 Pb Te 46.124(18) 1_545 . ?
OH4 Pb Te 74.63(8) 2_655 . ?
O2 Pb Te 27.86(8) 1_445 . ?
Pb Pb Te 60.101(8) 2 . ?
Pb Pb Te 60.101(9) 3 . ?
O2 Pb Pb 136.16(15) 2_655 17 ?
OH5 Pb Pb 80.81(19) . 17 ?
Cl4 Pb Pb 47.95(5) . 17 ?
Cl4 Pb Pb 118.12(5) 3 17 ?
Cl3 Pb Pb 98.44(5) . 17 ?
Cl2 Pb Pb 45.567(5) . 17 ?
Cl4 Pb Pb 105.12(4) 2_655 17 ?
Cl4 Pb Pb 46.15(4) 18_545 17 ?
Cu2 Pb Pb 120.38(2) . 17 ?
Cu1 Pb Pb 167.671(18) 1_545 17 ?
OH4 Pb Pb 147.88(8) 2_655 17 ?
O2 Pb Pb 133.81(8) 1_445 17 ?
Pb Pb Pb 74.075(10) 2 17 ?
Pb Pb Pb 108.306(9) 3 17 ?
Te Pb Pb 132.384(11) . 17 ?
O1 Te O1 91.3(2) 3_455 1_545 ?
```

```
O1 Te O1 91.3(2) 3_455 2_665 ?
O1 Te O1 91.3(2) 1_545 2_665 ?
O1 Te O2 178.4(3) 3_455 2_655 ?
O1 Te O2 88.4(2) 1_545 2_655 ?
O1 Te O2 87.1(2) 2_665 2_655 ?
O1 Te O2 87.1(2) 3_455 3_565 ?
O1 Te O2 178.4(2) 1_545 3_565 ?
O1 Te O2 88.4(2) 2_665 3_565 ?
O2 Te O2 93.2(2) 2_655 3_565 ?
O1 Te O2 88.4(2) 3_455 1_445 ?
O1 Te O2 87.1(2) 1_545 1_445 ?
O1 Te O2 178.4(2) 2_665 1_445 ?
O2 Te O2 93.2(2) 2_655 1_445 ?
O2 Te O2 93.2(2) 3_565 1_445 ?
O1 Te Cu2 138.57(18) 3_455 . ?
O1 Te Cu2 81.79(18) 1_545 . ?
O1 Te Cu2 48.40(18) 2_665 . ?
O2 Te Cu2 39.81(17) 2_655 . ?
O2 Te Cu2 99.24(18) 3_565 . ?
O2 Te Cu2 131.50(18) 1_445 . ?
O1 Te Cu2 81.79(18) 3_455 3 ?
O1 Te Cu2 48.41(18) 1_545 3 ?
O1 Te Cu2 138.57(17) 2_665 3 ?
O2 Te Cu2 99.24(18) 2_655 3 ?
O2 Te Cu2 131.50(18) 3_565 3 ?
O2 Te Cu2 39.81(17) 1_445 3 ?
Cu2 Te Cu2 119.887(3) . 3 ?
O1 Te Cu2 48.41(18) 3_455 2 ?
O1 Te Cu2 138.57(17) 1_545 2 ?
O1 Te Cu2 81.79(18) 2_665 2 ?
O2 Te Cu2 131.50(18) 2_655 2 ?
O2 Te Cu2 39.81(17) 3_565 2 ?
O2 Te Cu2 99.24(18) 1_445 2 ?
Cu2 Te Cu2 119.888(3) . 2 ?
Cu2 Te Cu2 119.888(3) 3 2 ?
O1 Te Cu1 35.31(17) 3_455 3_455 ?
O1 Te Cu1 94.51(18) 1_545 3_455 ?
O1 Te Cu1 126.31(18) 2_665 3_455 ?
O2 Te Cu1 146.32(17) 2_655 3_455 ?
O2 Te Cu1 84.34(18) 3_565 3_455 ?
O2 Te Cu1 53.62(18) 1_445 3_455 ?
Cu2 Te Cu1 173.14(4) . 3_455 ?
Cu2 Te Cu1 60.20(3) 3 3_455 ?
Cu2 Te Cu1 59.70(3) 2 3_455 ?
O1 Te Cu1 94.51(18) 3_455 2_665 ?
O1 Te Cu1 126.31(18) 1_545 2_665 ?
O1 Te Cu1 35.31(17) 2_665 2_665 ?
O2 Te Cu1 84.34(18) 2_655 2_665 ?
O2 Te Cu1 53.62(18) 3_565 2_665 ?
O2 Te Cu1 146.32(17) 1_445 2_665 ?
Cu2 Te Cu1 59.70(3) . 2_665 ?
Cu2 Te Cu1 173.14(4) 3 2_665 ?
Cu2 Te Cu1 60.20(3) 2 2_665 ?
Cu1 Te Cu1 119.270(8) 3_455 2_665 ?
O1 Te Cu1 126.31(18) 3_455 1_545 ?
```

```
O1 Te Cu1 35.31(17) 1_545 1_545 ?
O1 Te Cu1 94.51(18) 2_665 1_545 ?
O2 Te Cu1 53.62(18) 2_655 1_545 ?
O2 Te Cu1 146.32(17) 3_565 1_545 ?
O2 Te Cu1 84.34(18) 1_445 1_545 ?
Cu2 Te Cu1 60.20(3) . 1_545 ?
Cu2 Te Cu1 59.70(3) 3 1_545 ?
Cu2 Te Cu1 173.14(4) 2 1_545 ?
Cu1 Te Cu1 119.270(7) 3_455 1_545 ?
Cu1 Te Cu1 119.270(8) 2_665 1_545 ?
O1 Cu1 OH4 179.3(3) . 2_665 ?
O1 Cu1 OH3 98.3(3) . 1_565 ?
OH4 Cu1 OH3 81.3(2) 2_665 1_565 ?
O1 Cu1 OH4 87.1(2) . 3_565 ?
OH4 Cu1 OH4 93.3(3) 2_665 3_565 ?
OH3 Cu1 OH4 173.3(2) 1_565 3_565 ?
O1 Cu1 O2 72.9(2) . 2_665 ?
OH4 Cu1 O2 106.5(2) 2_665 2_665 ?
OH3 Cu1 O2 77.1(2) 1_565 2_665 ?
OH4 Cu1 O2 100.9(2) 3_565 2_665 ?
O1 Cu1 Cl1 93.96(17) . . ?
OH4 Cu1 Cl1 86.68(17) 2_665 . ?
OH3 Cu1 Cl1 97.39(18) 1_565 . ?
OH4 Cu1 Cl1 86.14(17) 3_565 . ?
O2 Cu1 Cl1 164.53(13) 2_665 . ?
OH3 Cu2 OH4 175.0(3) . . ?
OH3 Cu2 OH3 95.2(4) . 3_665 ?
OH4 Cu2 OH3 80.4(2) . 3_665 ?
OH3 Cu2 O2 89.9(3) . 2_655 ?
OH4 Cu2 O2 94.9(2) . 2_655 ?
OH3 Cu2 O2 169.3(2) 3_665 2_655 ?
OH3 Cu2 O1 103.4(2) . 2_665 ?
OH4 Cu2 O1 76.6(2) . 2_665 ?
OH3 Cu2 O1 114.0(2) 3_665 2_665 ?
O2 Cu2 O1 73.7(2) 2_655 2_665 ?
OH3 Cu2 Cl3 84.73(18) . . ?
OH4 Cu2 Cl3 97.02(17) . . ?
OH3 Cu2 Cl3 84.08(18) 3_665 . ?
O2 Cu2 Cl3 87.04(17) 2_655 . ?
O1 Cu2 Cl3 158.89(15) 2_665 . ?
Cu1 Cl1 Cu1 72.98(3) 13_565 14_455 ?
Cu1 Cl1 Cu1 72.98(4) 13_565 15 ?
Cu1 Cl1 Cu1 72.98(3) 14_455 15 ?
Cu1 Cl1 Cu1 180.0 13_565 . ?
Cu1 Cl1 Cu1 107.02(3) 14_455 . ?
Cu1 Cl1 Cu1 107.02(3) 15 . ?
Cu1 Cl1 Cu1 107.03(4) 13_565 3_565 ?
Cu1 Cl1 Cu1 107.02(4) 14_455 3_565 ?
Cu1 Cl1 Cu1 180.0 15 3_565 ?
Cu1 Cl1 Cu1 72.97(3) . 3_565 ?
Cu1 Cl1 Cu1 107.02(3) 13_565 2_665 ?
Cu1 Cl1 Cu1 180.0 14_455 2_665 ?
Cu1 Cl1 Cu1 107.02(3) 15 2_665 ?
Cu1 Cl1 Cu1 72.97(4) . 2_665 ?
Cu1 Cl1 Cu1 72.97(3) 3_565 2_665 ?
```

```
Cu1 Cl1 Cu2 78.32(3) 13_565 . ?
Cu1 Cl1 Cu2 131.28(3) 14_455 . ?
Cu1 Cl1 Cu2 133.46(3) 15 . ?
Cu1 Cl1 Cu2 101.68(3) . . ?
Cu1 Cl1 Cu2 46.54(3) 3_565 . ?
Cu1 Cl1 Cu2 48.72(3) 2_665 . ?
Cu1 Cl1 Cu2 48.72(3) 13_565 15 ?
Cu1 Cl1 Cu2 46.54(3) 14_455 15 ?
Cu1 Cl1 Cu2 101.68(3) 15 15 ?
Cu1 Cl1 Cu2 131.28(3) . 15 ?
Cu1 Cl1 Cu2 78.32(3) 3_565 15 ?
Cu1 Cl1 Cu2 133.46(3) 2_665 15 ?
Cu2 Cl1 Cu2 85.04(2) . 15 ?
Cu1 Cl1 Cu2 46.54(3) 13_565 14_455 ?
Cu1 Cl1 Cu2 101.68(3) 14_455 14_455 ?
Cu1 Cl1 Cu2 48.72(3) 15 14_455 ?
Cu1 Cl1 Cu2 133.46(3) . 14_455 ?
Cu1 Cl1 Cu2 131.28(3) 3_565 14_455 ?
Cu1 Cl1 Cu2 78.32(3) 2_665 14_455 ?
Cu2 Cl1 Cu2 85.04(2) . 14_455 ?
Cu2 Cl1 Cu2 94.96(2) 15 14_455 ?
Cu1 Cl1 Cu2 133.46(3) 13_565 2_665 ?
Cu1 Cl1 Cu2 78.32(3) 14_455 2_665 ?
Cu1 Cl1 Cu2 131.28(3) 15 2_665 ?
Cu1 Cl1 Cu2 46.54(3) . 2_665 ?
Cu1 Cl1 Cu2 48.72(3) 3_565 2_665 ?
Cu1 Cl1 Cu2 101.68(3) 2_665 2_665 ?
Cu2 Cl1 Cu2 94.96(2) . 2_665 ?
Cu2 Cl1 Cu2 85.04(2) 15 2_665 ?
Cu2 Cl1 Cu2 180.00(2) 14_455 2_665 ?
Cu1 Cl1 Cu2 131.28(3) 13_565 3_565 ?
Cu1 Cl1 Cu2 133.46(3) 14_455 3_565 ?
Cu1 Cl1 Cu2 78.32(3) 15 3_565 ?
Cu1 Cl1 Cu2 48.72(3) . 3_565 ?
Cu1 Cl1 Cu2 101.68(3) 3_565 3_565 ?
Cu1 Cl1 Cu2 46.54(3) 2_665 3_565 ?
Cu2 Cl1 Cu2 94.96(2) . 3_565 ?
Cu2 Cl1 Cu2 180.0 15 3_565 ?
Cu2 Cl1 Cu2 85.04(2) 14_455 3_565 ?
Cu2 Cl1 Cu2 94.96(2) 2_665 3_565 ?
Cu1 Cl1 Cu2 101.68(3) 13_565 13_565 ?
Cu1 Cl1 Cu2 48.72(3) 14_455 13_565 ?
Cu1 Cl1 Cu2 46.54(3) 15 13_565 ?
Cu1 Cl1 Cu2 78.32(3) . 13_565 ?
Cu1 Cl1 Cu2 133.46(3) 3_565 13_565 ?
Cu1 Cl1 Cu2 131.28(3) 2_665 13_565 ?
Cu2 Cl1 Cu2 180.00(2) . 13_565 ?
Cu2 Cl1 Cu2 94.96(2) 15 13_565 ?
Cu2 Cl1 Cu2 94.96(2) 14_455 13_565 ?
Cu2 Cl1 Cu2 85.04(2) 2_665 13_565 ?
Cu2 Cl1 Cu2 85.04(2) 3_565 13_565 ?
Pb Cl2 Pb 91.139(11) 17 16_655 ?
Pb Cl2 Pb 91.139(11) 17 18_545 ?
Pb Cl2 Pb 91.138(11) 16_655 18_545 ?
Pb Cl2 Pb 88.863(11) 17 . ?
```

```
Pb Cl2 Pb 180.0 16_655 . ?
Pb Cl2 Pb 88.863(11) 18_545 . ?
Pb Cl2 Pb 180.0 17 2_655 ?
Pb Cl2 Pb 88.863(11) 16_655 2_655 ?
Pb Cl2 Pb 88.863(11) 18_545 2_655 ?
Pb Cl2 Pb 91.135(11) . 2_655 ?
Pb Cl2 Pb 88.864(11) 17 3_665 ?
Pb Cl2 Pb 88.864(11) 16_655 3_665 ?
Pb Cl2 Pb 180.0 18_545 3_665 ?
Pb Cl2 Pb 91.135(11) . 3_665 ?
Pb Cl2 Pb 91.134(11) 2_655 3_665 ?
Cu2 Cl3 Cu2 75.78(9) 2_655 3_665 ?
Cu2 Cl3 Cu2 75.78(9) 2_655 . ?
Cu2 Cl3 Cu2 75.78(9) 3_665 . ?
Cu2 Cl3 Pb 81.05(3) 2_655 2_655 ?
Cu2 Cl3 Pb 107.55(3) 3_665 2_655 ?
Cu2 Cl3 Pb 155.02(7) . 2_655 ?
Cu2 Cl3 Pb 155.02(7) 2_655 3_665 ?
Cu2 Cl3 Pb 81.05(3) 3_665 3_665 ?
Cu2 Cl3 Pb 107.55(3) . 3_665 ?
Pb Cl3 Pb 97.39(7) 2_655 3_665 ?
Cu2 Cl3 Pb 107.55(3) 2_655 . ?
Cu2 Cl3 Pb 155.02(7) 3_665 . ?
Cu2 Cl3 Pb 81.05(3) . . ?
Pb Cl3 Pb 97.39(7) 2_655 . ?
Pb Cl3 Pb 97.39(7) 3_665 . ?
Cu2 Cl3 Cu1 47.27(4) 2_655 1_545 ?
Cu2 Cl3 Cu1 105.00(10) 3_665 1_545 ?
Cu2 Cl3 Cu1 50.02(4) . 1_545 ?
Pb Cl3 Cu1 106.533(18) 2_655 1_545 ?
Pb Cl3 Cu1 151.817(17) 3_665 1_545 ?
Pb Cl3 Cu1 65.39(2) . 1_545 ?
Cu2 Cl3 Cu1 50.02(4) 2_655 2_765 ?
Cu2 Cl3 Cu1 47.27(4) 3_665 2_765 ?
Cu2 Cl3 Cu1 105.00(10) . 2_765 ?
Pb Cl3 Cu1 65.39(2) 2_655 2_765 ?
Pb Cl3 Cu1 106.533(19) 3_665 2_765 ?
Pb Cl3 Cu1 151.817(17) . 2_765 ?
Cu1 Cl3 Cu1 96.99(6) 1_545 2_765 ?
Cu2 Cl3 Cu1 105.00(10) 2_655 3_565 ?
Cu2 Cl3 Cu1 50.02(4) 3_665 3_565 ?
Cu2 Cl3 Cu1 47.27(4) . 3_565 ?
Pb Cl3 Cu1 151.817(18) 2_655 3_565 ?
Pb Cl3 Cu1 65.39(2) 3_665 3_565 ?
Pb Cl3 Cu1 106.533(18) . 3_565 ?
Cu1 Cl3 Cu1 96.99(6) 1_545 3_565 ?
Cu1 Cl3 Cu1 96.99(6) 2_765 3_565 ?
Pb Cl4 Pb 87.60(7) . 2 ?
Pb Cl4 Pb 98.33(7) . 3_665 ?
Pb Cl4 Pb 164.83(9) 2 3_665 ?
Pb Cl4 Pb 93.65(7) . 17 ?
Pb Cl4 Pb 107.72(7) 2 17 ?
Pb Cl4 Pb 85.94(6) 3_665 17 ?
Pb Cl4 Cu2 62.33(5) . . ?
Pb Cl4 Cu2 93.42(6) 2 . ?
```

```
Pb Cl4 Cu2 77.26(5) 3_665 . ?
Pb Cl4 Cu2 147.63(7) 17 . ?
Pb Cl4 Cu1 93.05(6) . 2_665 ?
Pb Cl4 Cu1 63.05(4) 2 2_665 ?
Pb Cl4 Cu1 102.51(6) 3_665 2_665 ?
Pb Cl4 Cu1 168.35(8) 17 2_665 ?
Cu2 Cl4 Cu1 43.71(3) . 2_665 ?
Te O1 Cu1 109.6(3) 1_565 . ?
Te O1 Cu2 94.0(2) 1_565 3_565 ?
Cu1 O1 Cu2 93.3(2) . 3_565 ?
Te O1 Cu2 64.66(16) 1_565 1_565 ?
Cu1 O1 Cu2 64.97(17) . 1_565 ?
Cu2 O1 Cu2 138.8(2) 3_565 1_565 ?
Te O1 Cu2 117.2(2) 1_565 13_565 ?
Cu1 O1 Cu2 102.7(2) . 13_565 ?
Cu2 O1 Cu2 136.5(2) 3_565 13_565 ?
Cu2 O1 Cu2 84.02(13) 1_565 13_565 ?
Te O1 Cu1 55.34(14) 1_565 3_465 ?
Cu1 O1 Cu1 139.6(2) . 3_465 ?
Cu2 O1 Cu1 55.62(12) 3_565 3_465 ?
Cu2 O1 Cu1 119.74(15) 1_565 3_465 ?
Cu2 O1 Cu1 117.60(15) 13_565 3_465 ?
Te O1 Cu1 152.8(2) 1_565 15 ?
Cu1 O1 Cu1 96.8(2) . 15 ?
Cu2 O1 Cu1 90.95(17) 3_565 15 ?
Cu2 O1 Cu1 124.53(16) 1_565 15 ?
Cu2 O1 Cu1 47.56(7) 13_565 15 ?
Cu1 O1 Cu1 107.68(14) 3_465 15 ?
Te O1 Cu2 105.4(2) 1_565 15_455 ?
Cu1 O1 Cu2 143.7(2) . 15_455 ?
Cu2 O1 Cu2 93.81(17) 3_565 15_455 ?
Cu2 O1 Cu2 124.84(16) 1_565 15_455 ?
Cu2 O1 Cu2 50.95(8) 13_565 15_455 ?
Cu1 O1 Cu2 70.63(10) 3_465 15_455 ?
Cu1 O1 Cu2 47.58(7) 15 15_455 ?
Te O1 Cu1 131.4(2) 1_565 2_665 ?
Cu1 O1 Cu1 55.04(15) . 2_665 ?
Cu2 O1 Cu1 48.63(11) 3_565 2_665 ?
Cu2 O1 Cu1 119.87(15) 1_565 2_665 ?
Cu2 O1 Cu1 111.30(14) 13_565 2_665 ?
Cu1 O1 Cu1 103.92(14) 3_465 2_665 ?
Cu1 O1 Cu1 69.67(10) 15 2_665 ?
Cu2 O1 Cu1 106.72(13) 15_455 2_665 ?
Te O2 Cu2 103.2(2) 1_665 3_665 ?
Te O2 Pb 139.3(3) 1_665 3_665 ?
Cu2 O2 Pb 114.8(3) 3_665 3_665 ?
Te O2 Cu1 88.3(2) 1_665 3_565 ?
Cu2 O2 Cu1 85.9(2) 3_665 3_565 ?
Pb O2 Cu1 107.9(2) 3_665 3_565 ?
Te O2 Cu1 62.46(16) 1_665 1_655 ?
Cu2 O2 Cu1 61.59(15) 3_665 1_655 ?
Pb O2 Cu1 123.9(2) 3_665 1_655 ?
Cu1 O2 Cu1 126.26(19) 3_565 1_655 ?
Te O2 Cu2 51.72(14) 1_665 2_665 ?
Cu2 O2 Cu2 126.5(2) 3_665 2_665 ?
```

```
Pb O2 Cu2 109.67(19) 3_665 2_665 ?
Cu1 O2 Cu2 52.34(11) 3_565 2_665 ?
Cu1 O2 Cu2 113.94(15) 1_655 2_665 ?
Te O2 Pb 77.25(18) 1_665 1_665 ?
Cu2 O2 Pb 115.8(2) 3_665 1_665 ?
Pb O2 Pb 73.49(14) 3_665 1_665 ?
Cu1 O2 Pb 156.0(2) 3_565 1_665 ?
Cu1 O2 Pb 63.19(10) 1_655 1_665 ?
Cu2 O2 Pb 104.04(14) 2_665 1_665 ?
Te O2 Cu2 127.3(2) 1_665 . ?
Cu2 O2 Cu2 54.44(15) 3_665 . ?
Pb O2 Cu2 88.40(17) 3_665 . ?
Cu1 O2 Cu2 48.09(11) 3_565 . ?
Cu1 O2 Cu2 115.85(15) 1_655 . ?
Cu2 O2 Cu2 100.10(14) 2_665 . ?
Pb O2 Cu2 153.55(16) 1_665 . ?
Cu2 OH3 Cu1 106.3(3) . 1_545 ?
Cu2 OH3 Cu2 113.5(3) . 2_655 ?
Cu1 OH3 Cu2 99.0(3) 1_545 2_655 ?
Cu2 OH3 Cu2 63.40(17) . 3_665 ?
Cu1 OH3 Cu2 148.4(2) 1_545 3_665 ?
Cu2 OH3 Cu2 63.30(16) 2_655 3_665 ?
Cu2 OH3 Cu1 144.5(2) . 14_445 ?
Cu1 OH3 Cu1 91.7(2) 1_545 14_445 ?
Cu2 OH3 Cu1 92.8(2) 2_655 14_445 ?
Cu2 OH3 Cu1 114.03(15) 3_665 14_445 ?
Cu2 OH3 Cu1 146.4(2) . 3 ?
Cu1 OH3 Cu1 56.43(16) 1_545 3 ?
Cu2 OH3 Cu1 51.32(15) 2_655 3 ?
Cu2 OH3 Cu1 114.48(15) 3_665 3 ?
Cu1 OH3 Cu1 68.82(11) 14_445 3 ?
Cu2 OH3 Cu2 101.3(2) . 13 ?
Cu1 OH3 Cu2 92.3(2) 1_545 13 ?
Cu2 OH3 Cu2 138.2(2) 2_655 13 ?
Cu2 OH3 Cu2 118.57(16) 3_665 13 ?
Cu1 OH3 Cu2 46.48(7) 14_445 13 ?
Cu1 OH3 Cu2 107.49(15) 3 13 ?
Cu1 OH4 Cu2 99.3(3) 3_565 . ?
Cu1 OH4 Cu1 112.5(3) 3_565 2_665 ?
Cu2 OH4 Cu1 103.1(3) . 2_665 ?
Cu1 OH4 Cu1 63.48(16) 3_565 . ?
Cu2 OH4 Cu1 146.8(2) . . ?
Cu1 OH4 Cu1 63.39(15) 2_665 . ?
Cu1 OH4 Cu2 52.29(14) 3_565 3_665 ?
Cu2 OH4 Cu2 56.97(15) . 3_665 ?
Cu1 OH4 Cu2 144.7(2) 2_665 3_665 ?
Cu1 OH4 Cu2 115.63(15) . 3_665 ?
Cu1 OH4 Pb 74.75(17) 3_565 3_665 ?
Cu2 OH4 Pb 95.5(2) . 3_665 ?
Cu1 OH4 Pb 158.3(2) 2_665 3_665 ?
Cu1 OH4 Pb 105.74(14) . 3_665 ?
Cu2 OH4 Pb 56.20(8) 3_665 3_665 ?
Pb OH5 Pb 115.08(18) . 3 ?
Pb OH5 Pb 115.08(18) . 2 ?
Pb OH5 Pb 115.08(18) 3 2 ?
```

```
loop_
 _geom_hbond_atom_site_label_D
 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
 _geom_hbond_distance_HA
 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
OH3 H3 O1  0.89(2) 1.75(3) 2.634(8) 172(9) 14_445
OH4 H4 Cl4  0.90(2) 2.25(2) 3.144(6) 176(8) .
OH5 H5 Cl4  0.90(2) 2.737(16) 3.408(9) 132.5(4) 16
OH5 H5 Cl4  0.90(2) 2.737(16) 3.408(9) 132.5(4) 17_445
OH5 H5 Cl4  0.90(2) 2.737(16) 3.408(9) 132.5(4) 18_545

_diffrn_measured_fraction_theta_max    0.992
_diffrn_reflns_theta_full              25.02
_diffrn_measured_fraction_theta_full   0.992
_refine_diff_density_max    2.234
_refine_diff_density_min   -1.429
_refine_diff_density_rms    0.297
```

h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s
-1	2	0	294	302	3	-6	6	3	391	379	6	-9	6	6	82	88	8	2	5	9	384	373	16	-6	6	12	314	316	7
0	3	0	440	442	5	-3	6	3	689	696	28	-6	6	6	347	339	9	-9	6	9	73	79	24	-3	6	12	289	297	7
-2	4	0	417	404	7	0	6	3	46	44	7	-3	6	6	668	656	28	-6	6	9	146	154	9	0	6	12	218	210	8
-4	5	0	60	63	3	3	6	3	264	211	31	0	6	6	299	270	11	-3	6	9	180	183	7	3	6	12	50	68	19
-1	5	0	1313	1251	37	-8	7	3	13	29	13	3	6	6	89	109	22	0	6	9	477	485	27	-8	7	12	105	116	13
-3	6	0	247	238	5	-5	7	3	418	418	36	-8	7	6	54	74	8	3	6	9	610	582	29	-5	7	12	576	568	19
0	6	0	148	142	4	-2	7	3	144	135	6	-5	7	6	27	41	26	-8	7	9	217	221	4	-2	7	12	46	54	10
-5	7	0	739	726	26	1	7	3	238	235	11	-2	7	6	0	11	1	-5	7	9	230	238	8	1	7	12	131	130	6
-2	7	0	235	236	7	-7	8	3	68	67	7	1	7	6	199	222	9	-2	7	9	138	143	4	-7	8	12	254	268	5
-7	8	0	105	96	7	-4	8	3	35	32	34	-7	8	6	172	182	7	1	7	9	0	11	1	-4	8	12	52	69	14
-4	8	0	95	98	11	-1	8	3	137	139	8	-4	8	6	282	277	8	-7	8	9	184	193	6	-1	8	12	101	107	7
-1	8	0	202	214	9	-6	9	3	524	520	29	-1	8	6	154	156	4	-4	8	9	521	503	16	-6	9	12	150	159	6
-6	9	0	298	272	12	-3	9	3	11	37	10	-6	9	6	338	323	27	-1	8	9	4	27	4	-3	9	12	72	84	17
-3	9	0	174	182	15	-1	1	4	452	459	3	-3	9	6	119	121	7	-6	9	9	317	303	14	-1	1	13	71	65	3
-5	10	0	115	138	14	-3	2	4	180	178	2	-1	1	7	96	87	1	-3	9	9	214	209	8	-3	2	13	510	517	6
-3	2	1	201	213	4	0	2	4	669	676	8	-3	2	7	218	224	2	-1	1	10	189	187	2	0	2	13	649	655	8
0	2	1	468	468	5	-5	3	4	255	244	4	0	2	7	723	736	8	-3	2	10	538	536	6	-5	3	13	301	296	5
-5	3	1	70	63	6	-2	3	4	1184	1186	25	-5	3	7	82	86	4	0	2	10	59	50	4	-2	3	13	367	371	4
-2	3	1	1154	1142	28	1	3	4	406	400	5	-2	3	7	1389	1394	33	-5	3	10	362	363	5	1	3	13	499	504	6
1	3	1	738	731	9	-7	4	4	347	337	7	1	3	7	374	367	6	-2	3	10	138	124	3	-7	4	13	330	324	10
-7	4	1	237	252	12	-4	4	4	269	272	3	-7	4	7	440	439	17	1	3	10	532	530	6	-4	4	13	379	375	5
-4	4	1	327	323	4	-1	4	4	519	511	8	-4	4	7	137	132	3	-7	4	10	16	8	16	-1	4	13	433	429	6
-1	4	1	250	244	4	2	4	4	602	629	37	-1	4	7	824	821	12	-4	4	10	158	162	2	2	4	13	205	203	4
2	4	1	232	237	12	-9	5	4	134	152	14	2	4	7	603	560	35	-1	4	10	875	869	14	-9	5	13	146	128	13
-9	5	1	240	246	13	-6	5	4	366	363	4	-9	5	7	257	264	15	2	4	10	555	556	15	-6	5	13	392	389	9
-6	5	1	570	558	8	-3	5	4	413	409	7	-6	5	7	149	146	3	-9	5	10	143	146	13	-3	5	13	486	475	7
-3	5	1	348	330	8	0	5	4	565	557	12	-3	5	7	422	424	5	-6	5	10	387	384	7	0	5	13	381	382	10
0	5	1	332	334	4	3	5	4	123	135	7	0	5	7	500	475	11	-3	5	10	47	40	7	3	5	13	53	49	16
3	5	1	121	124	8	-8	6	4	307	303	21	3	5	7	55	68	14	0	5	10	83	94	10	-8	6	13	263	259	12
-8	6	1	117	114	8	-5	6	4	324	333	11	-8	6	7	504	445	75	3	5	10	30	23	29	-5	6	13	62	63	4
-5	6	1	134	132	4	-2	6	4	404	394	10	-5	6	7	90	89	5	-8	6	10	494	477	26	-2	6	13	257	256	5
-2	6	1	503	479	9	1	6	4	256	239	9	-2	6	7	346	335	6	-5	6	10	246	252	4	1	6	13	142	145	6
1	6	1	40	19	12	-7	7	4	133	134	5	1	6	7	265	254	14	-2	6	10	245	242	4	-7	7	13	410	405	10
-7	7	1	185	172	10	-4	7	4	225	223	9	-7	7	7	780	778	16	1	6	10	234	218	9	-4	7	13	26	25	9
-4	7	1	171	167	9	-1	7	4	133	127	5	-4	7	7	39	39	16	-7	7	10	244	263	7	-1	7	13	104	109	6
-1	7	1	33	44	10	2	7	4	249	189	29	-1	7	7	121	118	5	-4	7	10	26	20	26	2	7	13	288	267	14
2	7	1	159	159	14	-9	8	4	70	78	12	2	7	7	482	457	18	-1	7	10	124	138	6	-6	8	13	21	13	20
-9	8	1	265	214	25	-6	8	4	252	285	16	-9	8	7	124	129	11	2	7	10	70	61	15	-3	8	13	274	274	10
-6	8	1	155	163	12	-3	8	4	349	326	16	-6	8	7	0	35	1	-6	8	10	101	97	6	0	8	13	223	222	7
-3	8	1	46	22	15	0	8	4	182	189	9	-3	8	7	345	332	15	-3	8	10	527	502	19	-5	9	13	314	300	10
0	8	1	310	316	11	-8	9	4	24	34	24	0	8	7	233	235	8	0	8	10	237	232	13	-2	9	13	215	220	19
-8	9	1	40	38	28	-5	9	4	388	390	22	-8	9	7	24	21	24	-5	9	10	0	21	1	0	1	14	347	344	4
-5	9	1	285	265	17	-2	9	4	49	58	24	-5	9	7	317	318	14	-2	9	10	154	146	10	-2	2	14	371	369	3
-2	9	1	124	134	14	0	1	5	231	240	2	-2	9	7	0	20	1	0	1	11	194	199	2	1	2	14	106	98	4
-2	2	2	91	80	2	-2	2	5	742	762	8	0	1	8	266	274	2	-2	2	11	290	296	2	-4	3	14	899	900	15
-4	3	2	830	815	11	1	2	5	882	902	11	-2	2	8	775	784	9	1	2	11	1170	1187	22	-1	3	14	512	514	6
-1	3	2	466	458	7	-4	3	5	946	955	15	1	2	8	478	481	4	-4	3	11	145	141	3	2	3	14	93	94	5
2	3	2	30	21	11	-1	3	5	438	436	4	-4	3	8	450	454	7	-1	3	11	68	68	4	-6	4	14	179	181	6
-6	4	2	211	208	9	2	3	5	279	271	4	-1	3	8	158	153	3	2	3	11	282	284	3	-3	4	14	219	223	3
-3	4	2	481	477	6	-6	4	5	329	326	6	2	3	8	458	461	5	-6	4	11	545	533	14	0	4	14	312	308	5
0	4	2	69	68	3	-3	4	5	432	427	5	-6	4	8	219	225	11	-3	4	11	833	827	13	3	4	14	79	82	8
3	4	2	51	48	12	0	4	5	172	166	5	-3	4	8	262	256	3	0	4	11	400	392	6	-8	5	14	692	645	20
-8	5	2	576	567	14	3	4	5	28	25	27	0	4	8	313	305	5	3	4	11	191	178	6	-5	5	14	96	103	5
-5	5	2	145	138	3	-8	5	5	163	168	6	3	4	8	131	120	7	-8	5	11	131	131	9	-2	5	14	407	401	7
-2	5	2	395	392	8	-5	5	5	336	329	5	-8	5	8	127	114	9	-5	5	11	353	363	5	1	5	14	467	459	13
1	5	2	291	285	7	-2	5	5	58	45	8	-5	5	8	606	583	9	-2	5	11	24	31	15	4	5	14	53	44	34
4	5	2	68	73	12	1	5	5	48	44	7	-2	5	8	22	9	10	1	5	11	285	276	9	-7	6	14	247	250	7
-7	6	2	115	120	4	4	5	5	160	163	13	1	5	8	198	207	8	4	5	11	359	313	14	-4	6	14	618	612	9
-4	6	2	557	558	18	-7	6	5	113	120	5	4	5	8	447	417	19	-7	6	11	99	96	5	-1	6	14	296	292	8
-1	6	2	428	417	6	-4	6	5	297	302	18	-7	6	8	20	12	19	-4	6	11	400	405	8	2	6	14	91	106	11
2	6	2	62	47	12	-1	6	5	178	169	4	-4	6	8	272	270	7	-1	6	11	632	621	15	-9	7	14	167	173	23
-9	7	2	106	108	15	2	6	5	84	81	13	-1	6	8	316	306	11	2	6	11	208	204	8	-6	7	14	164	170	4
-6	7	2	124	122	8	-9	7	5	83	79	15	2	6	8	176	178	11	-9	7	11	69	76	20	-3	7	14	139	143	4
-3	7	2	60	52	8	-6	7	5	370	387	14	-9	7	8	75	58	12	-6	7	11	60	61	6	0	7	14	468	465	22
0	7	2	348	333	18	-3	7	5	374	365	8	-6	7	8	254	234	22	-3	7	11	223	245	7	-5	8	14	36	26	15
-8	8	2	178	177	11	0	7	5	647	623	28	-3	7	8	427	433	12	0	7	11	60	43	15	-2	8	14	448	436	14
-5	8	2	113	114	6	-8	8	5	177	189	7	0	7	8	356	331	15	-8	8	11	316	320	9	-7	9	14	177	182	9
-2	8	2	407	426	30	-5	8	5	153	159	6	-8	8	8	82	83	11	-5	8	11	114	120	6	-4	9	14	0	49	1
1	8	2	89	85	11	-2	8	5	590	545	36	-5	8	8	119	106	7	-2	8	11	64	74	8	0	0	15	877	908	18
-7	9	2	111	119	8	1	8	5	83	72	11	-2	8	8	328	284	18	-7	9	11	124	120	12	1	1	15	46	37	5
-4	9	2	95	94	8	-7	9	5	390	419	20	1	8	8	28	13	27	-4	9	11	316	303	11	-1	2	15	665	680	8
-1	9	2	284	292	9	-4	9	5	250	228	11	-7	9	8	314	313	14	0	0	12	2375	2349	148	2	2	15	101	101	3
1	1	3	27	18	4	-1	9	5	33	32	33	-4	9	8	23	47	22	1	1	12	435	446	4	-3	3	15	92	88	3
-1	2	3	709	733	9	1	1	6	454	463	3	-1	9	8	33	27	33	-1	2	12	731	738	9	0	3	15	240	240	3
2	2	3	88	83	9	-1	2	6	570	586	5	0	0	9	319	323	4	2	2	12	279	286	4	3	3	15	99	103	6
-3	3	3	33	7	7	2	2	6	207	211	2	-1	2	9	74	69	2	-3	3	12	262	259	3	-5	4	15	102	104	4
0	3	3	302	297	3	-3	3	6	224	223	2	2	2	9	242	239	2	0	3	12	214	211	3	-2	4	15	341	336	5
3	3	3	167	171	15	0	3	6	198	194	3	-3	3	9	76	80	2	3	3	12	582	618	18	1	4	15	462	458	6
-5	4	3	550	538	6	3	3	6	543	541	9	0	3	9	96	91	3	-5	4	12	770	753	16	4	4	15	284	286	20
-2	4	3	359	368	8	-5	4	6	382	383	5	3	3	9	623	611	11	-2	4	12	98	91	4	-7	5	15	123	145	11
1	4	3	608	587	8	-2	4	6	152	147	4	-5	4	9	490	476	8	1	4	12	238	234	6	-4	5	15	148	145	6
4	4	3	393	384	14	1	4	6	558	536	10	-2	4	9	84	83	4	4	4	12	50	47	9	-1	5	15	140	142	4
-7	5	3	93	87	7	4	4	6	349	338	16	1	4	9	127	116	5	-7	5	12	149	145	9	2	5	15	407	416	19
-4	5	3	154	153	3	-7	5	6	52	44	10	4	4	9	27	29	26	-4	5	12	222	220	4	-9	6	15	180	162	13
-1	5	3	272	262	10	-4	5	6	491	485	7	-7	5	9	92	93	10	-1	5	12	747	727	12	-6	6	15	320	326	9
2	5	3	353	350	8	-1	5	6	51	29	8	-4	5	9	715	710	12	2	5	12	638	614	18	-3	6	15	542	549	18
-9	6	3	153	167	20	2	5	6	75	95	9	-1	5	9	771	739	13	-9	6	12	143	130	10	0	6	15	50	43	15

h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s
3	6	15	76	75	27	-5	7	18	99	105	5	-3	9	21	104	110	13	-3	5	25	245	258	6	0	4	29	256	252	6
-8	7	15	80	90	10	-2	7	18	0	12	1	-1	1	22	26	17	11	0	5	25	259	258	5	3	4	29	92	104	8
-5	7	15	403	400	8	1	7	18	239	248	12	-3	2	22	184	181	3	3	5	25	55	24	24	-8	5	29	138	134	15
-2	7	15	114	120	6	-7	8	18	170	165	12	0	2	22	200	196	4	-8	6	25	189	175	17	-5	5	29	123	132	7
1	7	15	189	192	8	-4	8	18	162	182	7	-5	3	22	213	213	6	-5	6	25	138	150	6	-2	5	29	129	135	5
-7	8	15	42	59	19	-1	8	18	243	257	14	-2	3	22	366	370	4	-2	6	25	217	213	7	1	5	29	161	169	5
-4	8	15	96	102	7	-6	9	18	411	437	26	1	3	22	628	631	9	1	6	25	44	45	11	-7	6	29	24	14	23
-1	8	15	74	74	11	-3	9	18	113	121	11	-7	4	22	107	115	8	-7	7	25	460	459	13	-4	6	29	53	33	10
-6	9	15	290	298	10	-1	1	19	285	268	6	-4	4	22	44	47	9	-4	7	25	78	84	9	-1	6	29	120	121	5
-3	9	15	73	66	17	-3	2	19	337	332	4	-1	4	22	622	626	10	-1	7	25	130	130	6	2	6	29	107	99	18
-1	1	16	180	182	2	0	2	19	488	491	5	2	4	22	163	170	3	-6	8	25	35	51	35	-6	7	29	240	237	11
-3	2	16	106	107	2	-5	3	19	135	135	5	-9	5	22	271	245	20	-3	8	25	328	353	22	-3	7	29	138	146	9
0	2	16	770	775	10	-2	3	19	908	895	13	-6	5	22	408	412	8	0	1	26	52	55	6	0	7	29	224	230	11
-5	3	16	106	102	5	1	3	19	154	151	4	-3	5	22	152	150	4	-2	2	26	51	44	6	-5	8	29	113	126	13
-2	3	16	1458	1448	35	-7	4	19	247	249	6	0	5	22	235	223	5	1	2	26	74	71	5	-2	8	29	439	431	22
1	3	16	296	297	4	-4	4	19	105	101	4	3	5	22	52	82	30	-4	3	26	447	443	6	0	0	30	196	199	6
-7	4	16	420	413	11	-1	4	19	729	721	12	-8	6	22	337	332	14	-1	3	26	98	98	5	1	1	30	236	239	4
-4	4	16	181	181	5	2	4	19	344	340	5	-5	6	22	101	106	8	2	3	26	80	80	5	-1	2	30	435	437	7
-1	4	16	395	397	6	-9	5	19	155	145	14	-2	6	22	304	311	9	-6	4	26	360	367	9	2	2	30	230	226	5
2	4	16	732	704	12	-6	5	19	56	57	7	1	6	22	82	87	8	-3	4	26	508	535	8	-3	3	30	92	82	4
-9	5	16	132	157	17	-3	5	19	234	236	4	-7	7	22	53	17	17	0	4	26	95	101	4	0	3	30	79	91	6
-6	5	16	242	246	8	0	5	19	401	391	6	-4	7	22	103	104	7	3	4	26	102	116	7	3	3	30	349	350	13
-3	5	16	573	571	9	3	5	19	47	52	39	-1	7	22	41	39	14	-8	5	26	420	413	19	-5	4	30	428	425	9
0	5	16	506	488	9	-8	6	19	539	510	25	-6	8	22	5	18	4	-5	5	26	59	56	8	-2	4	30	130	131	4
3	5	16	137	149	8	-2	6	19	122	121	6	-3	8	22	188	215	11	-2	5	26	123	130	7	1	4	30	382	377	7
-8	6	16	173	175	15	1	6	19	319	318	13	-5	9	22	113	117	11	1	5	26	123	137	5	4	4	30	362	359	24
-5	6	16	277	285	4	-7	7	19	630	647	17	0	1	23	163	157	3	-7	6	26	60	81	14	-7	5	30	34	10	33
-2	6	16	215	218	5	-4	7	19	147	157	6	-2	2	23	298	299	3	-4	6	26	347	359	9	-4	5	30	245	248	6
1	6	16	93	108	8	-1	7	19	34	27	19	1	2	23	1300	1283	31	-1	6	26	500	483	10	-1	5	30	140	147	6
-7	7	16	61	52	12	-6	8	19	73	99	9	-4	3	23	107	108	5	2	6	26	65	61	21	2	5	30	35	12	27
-4	7	16	78	92	6	-3	8	19	190	212	10	-1	3	23	75	77	4	-6	7	26	47	28	11	-6	6	30	240	245	8
-1	7	16	105	104	6	0	8	19	61	76	10	2	3	23	182	178	3	-3	7	26	0	23	1	-3	6	30	474	475	10
2	7	16	200	189	19	-5	9	19	275	274	10	-6	4	23	440	435	9	0	7	26	275	268	11	0	6	30	163	171	8
-6	8	16	250	271	8	0	1	20	215	216	3	-3	4	23	623	628	9	-5	8	26	139	172	12	-2	7	30	30	39	20
-3	8	16	361	393	11	-2	2	20	841	844	12	0	4	23	255	254	5	-2	8	26	235	249	13	-4	8	30	167	184	12
0	8	16	157	158	10	1	2	20	91	91	5	3	4	23	124	131	6	0	0	27	1016	1044	29	-1	1	31	153	152	3
-5	9	16	317	325	10	-4	3	20	380	382	6	-8	5	23	236	231	19	1	1	27	243	243	3	-3	2	31	240	239	5
-2	9	16	58	59	16	-1	3	20	61	57	5	-5	5	23	270	276	5	-1	2	27	469	478	6	0	2	31	366	367	7
0	1	17	303	310	3	2	3	20	435	429	5	-2	5	23	73	82	8	2	2	27	305	291	7	-5	3	31	97	94	7
-2	2	17	575	574	6	-6	4	20	85	89	6	1	5	23	225	221	5	-3	3	27	158	164	3	-2	3	31	339	340	5
1	2	17	810	814	11	-3	4	20	68	68	5	4	5	23	267	246	14	0	3	27	448	447	6	1	3	31	43	33	11
-4	3	17	913	902	17	0	4	20	232	233	4	-7	6	23	96	94	9	3	3	27	50	50	9	-7	4	31	197	197	13
-1	3	17	339	341	4	3	4	20	65	63	7	-4	6	23	507	524	16	-5	4	27	190	189	5	-4	4	31	49	56	9
2	3	17	230	229	4	-8	5	20	74	62	19	-1	6	23	547	547	11	-2	4	27	322	340	7	-1	4	31	574	556	10
-6	4	17	221	229	7	-5	5	20	537	540	10	2	6	23	191	170	12	1	4	27	272	269	5	2	4	31	98	107	4
-3	4	17	281	283	4	-2	5	20	106	99	5	-6	7	23	170	180	8	4	4	27	91	111	19	-6	5	31	80	75	9
0	4	17	186	183	3	1	5	20	40	28	11	-3	7	23	201	215	7	-7	5	27	221	229	13	-3	5	31	202	214	7
3	4	17	76	80	8	4	5	20	412	381	23	0	7	23	89	87	10	-4	5	27	236	237	5	0	5	31	328	328	9
-8	5	17	37	36	37	-7	6	20	164	169	16	-5	8	23	91	99	9	-1	5	27	390	386	10	3	5	31	55	60	17
-5	5	17	287	286	5	-4	6	20	21	30	20	-2	8	23	35	21	23	2	5	27	470	482	14	-5	6	31	205	207	6
-2	5	17	64	70	6	-1	6	20	170	174	6	-4	9	23	281	263	11	-6	6	27	175	176	6	-2	6	31	125	123	7
1	5	17	92	86	7	2	6	20	55	77	10	0	0	24	1417	1445	53	-3	6	27	294	311	8	1	6	31	256	257	11
4	5	17	150	143	15	-6	7	20	175	183	11	1	1	24	256	264	3	0	6	27	83	98	6	-7	7	31	426	424	12
-7	6	17	104	97	7	-3	7	20	435	434	13	-1	2	24	469	475	5	-5	7	27	474	483	15	-4	7	31	132	150	9
-4	6	17	161	172	4	0	7	20	490	476	16	2	2	24	348	333	5	-2	7	27	116	119	7	-1	7	31	81	70	8
-1	6	17	174	174	5	-8	8	20	29	34	28	-3	3	24	174	182	3	-4	8	27	129	148	14	-3	8	31	56	52	12
2	6	17	64	80	7	-5	8	20	57	78	12	0	3	24	239	235	4	-1	1	28	408	411	5	0	1	32	115	113	5
-9	7	17	91	78	14	-2	8	20	241	233	12	3	3	24	489	487	13	-3	2	28	169	169	4	-2	2	32	672	670	11
-6	7	17	288	287	8	-4	9	20	53	50	19	-5	4	24	435	433	7	0	2	28	509	510	7	1	2	32	436	429	7
-3	7	17	243	255	8	0	0	21	155	171	6	-2	4	24	157	157	4	-5	3	28	192	199	6	-4	3	32	376	365	6
0	7	17	465	457	15	1	1	21	770	773	10	1	4	24	195	191	4	-2	3	28	1109	1105	21	-1	3	32	22	12	21
-8	8	17	82	94	11	-1	2	21	144	133	3	4	4	24	26	46	25	1	3	28	386	378	6	2	3	32	453	428	9
-5	8	17	148	146	10	2	2	21	71	64	4	-7	5	24	148	174	8	-7	4	28	274	290	9	-6	4	32	64	52	12
-2	8	17	513	480	15	-3	3	21	35	31	5	-4	5	24	201	218	5	-4	4	28	34	20	19	-3	4	32	67	75	7
-7	9	17	330	311	12	0	3	21	414	407	5	-1	5	24	409	402	8	-1	4	28	472	472	9	0	4	32	103	110	6
-4	9	17	140	139	9	3	3	21	445	454	10	2	5	24	553	575	16	2	4	28	617	598	10	3	4	32	36	30	18
0	0	18	187	197	5	-5	4	21	371	372	6	-6	6	24	198	200	7	-6	5	28	348	349	8	-5	5	32	407	410	9
1	1	18	256	255	3	-2	4	21	36	32	9	-3	6	24	121	125	5	-3	5	28	480	483	8	-2	5	32	148	155	5
-1	2	18	611	618	6	1	4	21	69	56	6	0	6	24	210	196	5	0	5	28	267	265	6	1	5	32	18	23	17
2	2	18	332	330	3	4	4	21	136	149	10	-8	7	24	71	74	15	3	5	28	226	225	22	-7	6	32	202	197	12
-3	3	18	327	320	4	-7	5	21	40	69	16	-5	7	24	482	499	18	-8	6	28	72	62	18	-4	6	32	239	243	7
0	3	18	50	53	5	-4	5	21	750	763	12	-2	7	24	32	23	19	-5	6	28	322	318	7	-1	6	32	71	77	7
3	3	18	472	476	10	-1	5	21	645	625	11	1	7	24	93	90	11	-2	6	28	326	308	9	-6	7	32	87	94	9
-5	4	18	514	507	7	2	5	21	270	266	7	-7	8	24	194	196	9	1	6	28	44	20	12	-3	7	32	421	415	13
-2	4	18	79	78	5	-9	6	21	137	127	17	-4	8	24	116	132	7	-7	7	28	88	87	10	0	0	33	75	79	10
1	4	18	573	552	9	-6	6	21	122	123	9	-1	8	24	106	96	9	-4	7	28	79	89	10	1	1	33	446	447	7
4	4	18	401	382	17	-3	6	21	180	189	6	-1	1	25	30	21	9	-1	7	28	112	121	8	-1	2	33	310	314	5
-7	5	18	60	57	12	0	6	21	446	438	14	-3	2	25	306	302	4	-6	8	28	259	278	18	2	2	33	199	197	6
-4	5	18	300	309	6	3	6	21	603	544	26	0	2	25	508	500	8	-3	8	28	365	390	25	-3	3	33	179	181	5
-1	5	18	153	153	4	-8	7	21	256	248	13	-5	3	25	286	280	6	0	1	29	318	315	5	0	3	33	140	138	5
2	5	18	105	113	8	-5	7	21	81	91	7	-2	3	25	103	99	4	-2	2	29	358	357	6	3	3	33	289	278	9
-9	6	18	44	21	39	-2	7	21	166	173	6	1	3	25	435	425	6	1	2	29	392	381	6	-5	4	33	143	140	6
-6	6	18	350	344	10	1	7	21	45	47	16	-7	4	25	180	200	8	-4	3	29	796	768	15	-2	4	33	121	129	6
-3	6	18	608	608	24	-7	8	21	196	210	9	-4	4	25	217	220	5	-1	3	29	270	276	5	1	4	33	198	195	5
0	6	18	153	137	8	-4	8	21	498	516	22	-1	4	25	412	417	7	2	3	29	186	179	4	-7	5	33	93	107	10
3	6	18	55	69	30	-1	8	21	97	126	13	2	4	25	327	327	7	-6	4	29	134	143	7	-4	5	33	501	481	10
-8	7	18	0	26	1	-6	9	21	256	252	13	-6	5	25	303	315	7	-3	4	29	159	162	4	-1	5	33	372	358	8

h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s	h	k	l	Fo	Fc	s
2	5	33	281	274	17	1	1	36	384	385	6	-3	4	38	354	359	7	-3	4	41	61	67	10	-3	3	45	142	144	6
-6	6	33	231	233	11	-1	2	36	402	398	8	0	4	38	78	82	8	0	4	41	208	208	9	0	3	45	39	47	21
-3	6	33	220	220	6	2	2	36	97	103	6	-5	5	38	45	39	15	-5	5	41	57	65	15	-5	4	45	40	30	30
0	6	33	218	224	10	-3	3	36	20	27	20	-2	5	38	133	138	7	-2	5	41	224	233	7	-2	4	45	104	106	8
-5	7	33	191	201	8	0	3	36	58	60	10	1	5	38	129	134	8	-4	6	41	203	202	13	1	4	45	151	172	10
-2	7	33	253	239	8	3	3	36	452	446	16	-4	6	38	213	226	11	0	0	42	293	282	12	-4	5	45	342	326	9
-1	1	34	110	111	5	-5	4	36	75	72	9	-1	6	38	414	403	9	1	1	42	166	161	6	-1	5	45	190	198	10
-3	2	34	116	120	6	-2	4	36	53	42	10	0	0	39	936	913	35	-1	2	42	389	390	8	-1	1	46	110	122	8
0	2	34	224	228	5	1	4	36	257	251	7	1	1	39	140	132	6	2	2	42	126	120	7	-3	2	46	76	76	10
-5	3	34	74	81	9	-7	5	36	57	64	16	-1	2	39	415	423	10	-3	3	42	120	124	6	0	2	46	136	133	8
-2	3	34	427	436	8	-4	5	36	369	358	8	2	2	39	194	184	7	0	3	42	46	19	17	-2	3	46	410	404	10
1	3	34	511	508	9	-1	5	36	36	30	23	-3	3	39	53	50	10	3	3	42	183	188	9	1	3	46	299	293	11
-7	4	34	142	147	9	2	5	36	366	371	18	0	3	39	239	229	6	-5	4	42	418	398	10	-4	4	46	77	79	12
-4	4	34	75	71	7	-6	6	36	192	205	11	3	3	39	30	2	30	-2	4	42	60	56	9	-1	4	46	312	306	9
-1	4	34	426	413	10	-3	6	36	175	177	7	-5	4	39	235	231	10	1	4	42	313	306	9	0	1	47	68	60	9
2	4	34	41	45	9	0	6	36	232	233	9	-2	4	39	214	216	6	-4	5	42	124	140	6	-2	2	47	299	294	8
-6	5	34	416	411	11	-5	7	36	296	277	10	1	4	39	300	288	8	-1	5	42	176	185	7	1	2	47	460	440	12
-3	5	34	165	168	7	-2	7	36	48	56	15	-4	5	39	85	106	7	-3	6	42	387	374	10	-4	3	47	138	144	9
0	5	34	222	223	7	-1	1	37	125	136	5	-1	5	39	372	366	9	-1	1	43	253	249	6	-1	3	47	54	42	12
-5	6	34	45	45	16	-3	2	37	108	116	6	-3	6	39	179	186	9	-3	2	43	144	149	7	-3	4	47	262	260	9
-2	6	34	378	365	9	0	2	37	293	290	7	-1	1	40	180	181	5	0	2	43	254	257	6	0	4	47	263	263	12
1	6	34	75	90	17	-5	3	37	360	364	8	-3	2	40	321	317	9	-5	3	43	159	166	11	0	0	48	255	250	13
-4	7	34	76	87	9	-2	3	37	47	54	10	0	2	40	623	607	14	-2	3	43	41	9	15	1	1	48	299	300	8
-1	7	34	10	10	10	1	3	37	394	393	10	-5	3	40	30	9	27	1	3	43	35	32	21	-1	2	48	214	213	7
0	1	35	135	141	5	-7	4	37	149	152	8	-2	3	40	495	486	10	-4	4	43	60	55	13	2	2	48	71	83	11
-2	2	35	277	285	5	-4	4	37	143	159	6	1	3	40	117	122	6	-1	4	43	496	482	11	-3	3	48	51	45	13
1	2	35	968	935	22	-1	4	37	379	378	9	-4	4	40	79	84	9	-3	5	43	134	143	8	0	3	48	19	28	18
-4	3	35	86	85	6	2	4	37	307	301	13	-1	4	40	160	160	7	0	5	43	180	180	8	-2	4	48	0	24	1
-1	3	35	48	53	8	-6	5	37	198	193	11	2	4	40	235	224	10	0	1	44	173	184	6	-1	1	49	42	51	20
2	3	35	93	92	7	-3	5	37	118	121	6	-6	5	40	184	185	8	-2	2	44	524	517	12	-3	2	49	53	37	19
-6	4	35	349	348	12	0	5	37	200	202	7	-3	5	40	512	515	15	1	2	44	292	302	11	0	2	49	123	116	9
-3	4	35	424	425	8	-5	6	37	121	122	9	0	5	40	269	268	7	-4	3	44	354	351	10	-2	3	49	46	48	16
0	4	35	215	228	8	-2	6	37	78	60	10	-5	6	40	47	54	15	-1	3	44	0	17	1	0	1	50	134	140	8
3	4	35	101	113	7	-4	7	37	75	79	9	-2	6	40	142	143	7	2	3	44	357	335	12	-2	2	50	32	45	32
-5	5	35	288	284	9	0	1	38	49	42	9	0	1	41	333	324	7	-3	4	44	0	11	1	1	2	50	251	243	11
-2	5	35	69	71	9	-2	2	38	72	82	7	-2	2	41	143	140	6	0	4	44	85	91	10	-1	3	50	50	33	19
1	5	35	107	111	6	1	2	38	98	105	7	1	2	41	50	61	12	-2	5	44	68	68	9	0	0	51	694	658	30
-4	6	35	427	455	16	-4	3	38	360	351	8	-4	3	41	652	621	13	0	0	45	72	57	26	1	1	51	75	85	14
-1	6	35	397	388	9	-1	3	38	103	96	7	-1	3	41	221	219	8	1	1	45	313	309	8	-1	2	51	307	290	10
-3	7	35	138	124	8	2	3	38	16	7	16	2	3	41	60	66	12	-1	2	45	261	275	8	-1	1	52	122	135	10
0	0	36	616	611	18	-6	4	38	301	294	10	-6	4	41	26	29	26	2	2	45	183	181	9						