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Rickturnerite, $Pb_7O_4[Mg(OH)_4](OH)Cl_3$, a complex new lead oxychloride mineral

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ABSTRACT

Rickturnerite, which has the ideal formula $Pb_7O_4[Mg(OH)_4](OH)Cl_3$, is a new mineral from Torr Works (Merehead) quarry, near the village of Cranmore in Somerset, United Kingdom. It occurs as pale emerald green to grey porous aggregates of disordered interwoven minute fibrous crystals with mereheadite, cerussite, calcite, aragonite, mimetite, hydrocerussite, 'plumbonacrite' and an uncharacterized lead oxychloride, in cavities inside a manganite and pyrolusite pod. The crystals are typically less than 5 μm wide and 200 μm long, but they can reach 40 × 100 μm in cross-section and over 1 mm in length. The mineral is translucent with a vitreous lustre and each needle is brittle with an indistinct cleavage, breaking with a splintery fracture. The streak is white, the Mohs hardness ~3 and the density calculated using the empirical formula 6.886 g cm^{-3}. Electron microprobe analyses yielded PbO 87.7, MgO 1.79, CuO 0.14, Cl 6.62 wt.%; H_2O was calculated on the basis of structural considerations as 2.27 wt.% totalling 97.02 wt.%. A charge-balanced formula, based on 12 anions, is $Pb_{7.16}Mg_{0.81}Cu_{0.03}Cl_{3.40}H_{4.60}O_{8.60}$. Rickturnerite is orthorhombic *Pnma*, with a = 5.8024(6), b = 22.717(2), c = 25.879(3) Å, V = 3411.2(6) $Å^3$ and Z = 8. The diffraction pattern contains strong reflections that define a subcell with a = 5.8034(5), b = 11.3574(9), c = 12.939(2) Å, V = 852.9(6) $Å^3$ (space group *Pmm*2 which is related to the real unit cell by the transformation matrix [100/020/002]), and weak reflections that correspond to doubled b and c parameters. Since the difference between the large and small cells is only in a number of split and low-occupancy positions in the disordered region of the structure we provide the description of the subcell structure. The five strongest lines in the X-ray powder diffraction pattern [listed as d_{obs} (Å), I_{obs}, (*hkl*)] are as follows: 6.474, 100, (400); 3.233, 73, (107); 2.867, 57, (705); 5.636, 44, (011); 3.112, 31, (802). The crystal structure was solved by direct methods and refined using 1318 unique reflections to R_1 = 0.063. The structure is composed of a fully ordered part consisting of double $[O_2Pb_3]^{2+}$ chains of oxocentred $[OPb_4]$ tetrahedra extended along the b-axis, which together with Cl^- ions form 2-dimensional blocks parallel to (001). In between these blocks, there is a disordered region containing ordered $[Mg(OH)_6]^{4-}$ octahedra and low-occupancy Pb and OH sites with a slight degree of ordering; these produce the weak supercell reflections.

Keywords: rickturnerite, chloroxiphite, oxocentred tetrahedra, new mineral species, lead magnesium oxychloride, Merehead quarry, Somerset, mineral nomenclature, Torr Works quarry, new structure type.

Introduction

Rickturnerite was discovered by geologist and mineral collector Rick Turner in July 2005 when a group of three manganese pods containing rare lead oxychloride minerals were uncovered in Carboniferous limestone exposed on a belt

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decline leading down from Bench F at Torr Works (Merehead) quarry in Somerset, England, UK. An isolated region of the oxychloride assemblage in the largest pod contained an unusual green fibrous mineral. Specimens of the unknown phase were brought to the Natural History Museum (NHM) in London for identification, where preliminary analysis by X-ray diffraction (XRD) and energy-dispersive X-ray spectrometry (EDX) showed that it was a new species. After several years of research the material has been fully characterized and named rickturnerite, in honour of its discoverer. The new mineral and mineral name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (IMA 2010-034) and the holotype specimen is registered as BM 2008,100 at the NHM. A probe block (P15150) and several cotype specimens (with associated analytical data) are also registered at the NHM. Further analysed specimens are preserved in the private collection of Rick Turner; some of these have been dispersed to other museums for safekeeping.

Occurrence

Rickturnerite is a very rare constituent of the Pb-dominated mineral assemblage in the manganese oxide pods that are irregularly distributed in the Carboniferous limestone at Torr Works (Merehead) quarry (51º12′N 2º25′W) (Fig. 1). Associated minerals include mereheadite, cerussite, calcite, aragonite, mimetite, hydrocerussite, 'plumbonacrite' and an uncharacterized lead oxychloride, all of which are occur in cavities in the manganite and pyrolusite pods. The quarry is worked for aggregate; it is well known to geologists and mineral collectors for its unusual lead oxychloride mineral assemblage (Symes and Embrey, 1977; Turner and Rumsey, 2010). The mineralization in the quarry and surrounding area is of considerable scientific importance as it includes the type localities for the rare minerals mendipite (Spencer, 1923), chloroxiphite (Spencer, 1923; Siidra *et al*., 2008*b*), diaboleite (Spencer, 1923), parkinsonite (Symes *et al*., 1994), mereheadite (Welch *et al*., 1998; Krivovichev *et al*., 2009) and symesite (Welch *et al*., 2000).

Physical and optical properties

Rickturnerite occurs as thin elongated fibres of a translucent pale emerald green colour (Fig. 2). The fibres are flattened in cross-section, they are generally <5 μm wide and can be up to 1 mm long, although most are broken and shorter at around 200 μm in length. The fibres occur most commonly in disordered, sometimes interwoven, porous aggregates up to 16 × 5 × 5 mm in partially filled cavities. Thicker aggregates of rickturnerite

FIG. 1. Map of the Mendips region after Din *et al*. (1986), highlighting the position of Merehead quarry (M in red) in relation to other deposits in the area, with an inset showing the location in the UK.

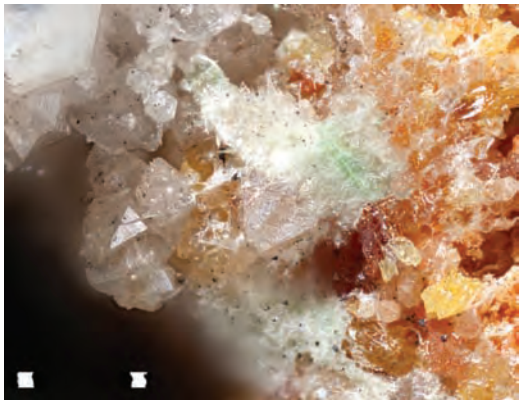


FIG. 2. Fibrous pale green to white rickturnerite on specimen BM2008,100 in the NHM collection; scale divisions are 1 mm.

fibres, up to 100×40 μm in cross-section and over 1 mm long are less common. These aggregates are darker green in colour and consist of a reinforced region of aligned, parallel and contiguous, thin, flat fibres that are identical to those in the rest of the mass. Rarely, the fibres grade into associated phases to produce anhedral dark green grains, which may be several millimetres across. The intensity of the green colour in hand specimen is determined by the thickness of the fibres in the aggregates. Rickturnerite is not fluorescent. It has a white streak, a vitreous lustre, a Mohs hardness of ~3 and an average VHN_{100} hardness of 140 kg mm^{-1}. The mineral has a visually splintery fracture, and the individual needles are brittle, bending only very slightly before fracturing, despite their elongated form. The splintery fracture is an artefact of the needle-like masses; the true parting and cleavage of individual crystals could not be assessed. The density could not be measured due to lack of sample; it was calculated as 6.886 g cm^{-3} on the basis of the unit cell and the empirical formula.

Rickturnerite is not metallic, but has a high refractive index (*RI*), which is typical of lead oxychlorides. The optical properties were studied using methods common for metallic minerals to avoid toxic refractive index liquids. In reflected light rickturnerite is grey, with weak bireflectance and no pleochroism; the samples studied had abundant greenish-grey internal reflections. Reflectance measurements were made using a SiC standard in air in the range 400–700 nm on a Zeiss Axiotron microscope. A crystal structures (Lanham) superstage was used to level the specimen and the standard prior to measurement with a J & M Tidas diode array spectrometer. Cavendish Instruments *Onyx* software produced data at intervals of 0.823 nm which were smoothed to give the data listed in Table 1. These are similar to other lead oxychlorides and were used to calculate mean *RI* values in air for rickturnerite at 589 nm using the Fresnel equation (Criddle, 1998) with the assumption that $k = 0$; this gave $R_1 = 2.17$ and $R_2 = 2.20$. These results are in good agreement with similar compounds, e.g. chloroxiphite *RI*s = 2.16, 2.24 and 2.25, mereheadite *RI*s = 2.19 and 2.28 and symesite *RI*s = 2.12 and 2.16 (Anthony *et al*., 2001).

TABLE 1. Measured reflectance values including COM standard wavelengths for rickturnerite.

R_1	R_2	λ (nm)	R_1	R_2	λ (nm)
16.5	17.7	400	13.7	14.3	560
16.1	17.1	420	13.6	14.2	580
15.5	16.4	440	13.6	14.2	589 (COM)
15.1	15.9	460	13.5	14.1	600
14.9	15.7	470 (COM)	13.4	14	620
14.7	15.4	480	13.4	14	640
14.3	15	500	13.4	14	650 (COM)
14	14.7	520	13.4	14.1	660
13.8	14.4	540	13.5	14.2	680
13.8	14.4	546 (COM)	13.6	14.3	700

Mean *RI* values in air at 589 nm calculated from the Fresnel equation (assuming $k = 0$) are $R_1 = 2.17$, $R_2 = 2.20$.

TABLE 2. Electron microprobe data for rickturnerite.

Constituent	Mean value (wt.%)	Range	SD	Standards
PbO	87.70	86.80–88.40	0.51	Vanadinite
MgO	1.79	1.63–1.99	0.12	Forsterite
CuO	0.14	0.10–0.16	0.02	Copper
Cl	6.62	6.43–6.88	0.12	Vanadinite
H_2O(calc)	2.27			
$O \equiv Cl$	−1.50			
Total	97.02			

Chemical composition

Rickturnerite aggregates were removed for chemical analysis from holotype and cotype specimens. The aggregates were mounted in epoxy, polished, carbon-coated and analysed using a Cameca SX100 electron microprobe at the NHM, operating in wavelength-dispersive (WDX) mode with an accelerating potential of 20 kV, probe current of 20 nA and a beam diameter of 20 μm. Water and peak overlap corrections were taken into account in the (PAP) matrix correction (Pouchou and Pichoir, 1988). The elements Pb, Mg, Cu and Cl were analysed; Mo, As, P, F, Cr, V and Si were sought but were below detection limits. No other elements were detected using EDX analysis on a variable pressure scanning electron microscope (JEOL 5900LV). Direct determination of H_2O was impossible due to a lack of sample; the H_2O content was calculated on the basis of the structural considerations outlined in the crystallography section. The absence of carbonate was confirmed by an uncoated EDX analysis on a scanning electron microscope (ZEISS LEO 1455VP) in low vacuum mode. Insufficient material exists for the determination of H_2O or CO_2 using a CHN analyser. Analytical results are given in Table 2.

The empirical formula (based on 12 anions) is $Pb_{7.16}Mg_{0.81}Cu_{0.03}Cl_{3.40}H_{4.60}O_{8.60}$. A combination of structural and chemical data is required to obtain an ideal formula. The crystallographic data (see below) reveal a disordered area of the structure that contains (Mg,Cu)$[OH]_6$ octahedra and irregularly distributed low-occupancy Pb and OH sites. There are hints of ordering of these Pb and OH sites, indicating the possible presence of a supercell, but characterization of this was beyond the scope of the project. The ideal endmember formula reported here based on subcell data is $Pb_7O_4[Mg(OH)_4](OH)Cl_3$, which requires PbO 90.31, MgO 2.33, Cl 6.15, H_2O 2.60, $O \equiv Cl$ −1.39, total 100.00 wt.%. The discrepancy between the ideal and empirical formulae is interpreted as reflecting the degree of disorder and irregularity in occupancy in the $Mg[OH]_6$, Pb and OH layer.

Crystallography

A single fibre was removed from a larger aggregate and mounted on a Stoe IPDS II Image-Plate based X-ray diffractometer operated at 50 kV and 40 mA at the Department of Crystallography, St Petersburg State University,

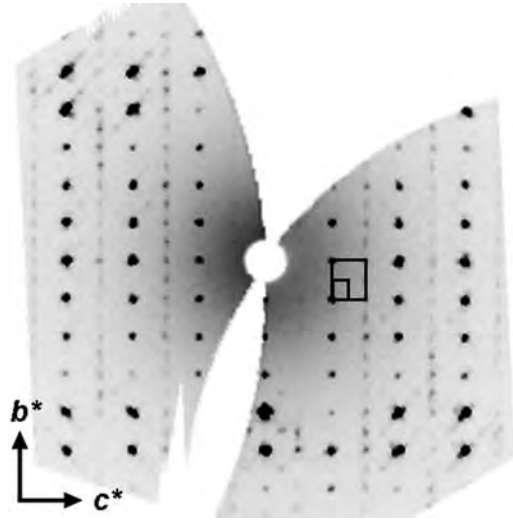


FIG. 3. The (100) section of reciprocal diffraction space containing both strong and weak reflections. The relation between subcell and supercell in the reciprocal lattice is shown.

Russia. More than a hemisphere of three-dimensional data were collected using monochromatic Mo$K\alpha$ radiation, with frame widths of 2º in ω, and a 360 s count time for each frame. The unit-cell parameters (Table 3) were refined using least-squares techniques. The analysis revealed orthorhombic symmetry with space group *Pnma*, $a = 5.8024(6)$, $b = 22.717(2)$, $c = 25.879(3)$ Å, $V = 3411.2(6)$ Å^3 and $Z = 8$. The diffraction pattern contains strong reflections that define a subcell with $a = 5.8034(5)$, $b = 11.3574(9)$, $c = 12.939(2)$ Å, and $V = 852.9(6)$ Å^3 (space group *Pmm*2 which is related to the real unit cell by the transformation matrix [100/020/002]) and weak reflections that correspond to doubled b and c parameters (Fig. 3). The intensity data were integrated and corrected for Lorentz, polarization and background effects using the Stoe program *X-area* (Stoe and Cie, 2007). Structure solution and parameter refinement (full-matrix least-squares on F^2) was performed using the *SHELX-97* software suite (Sheldrick, 2008).

Refinement in the large cell resulted in the rather high R value of 0.14, due to serious correlation problems in the ordered part of the structure. The refinement of the subcell structure was far more stable, especially in terms of the non-disordered structure fragments. Since the difference between the large and small cells is in a number of split and low-occupancy positions in the disordered region of the structure only (see below), here we provide the description of the subcell structure; a complete crystallographic description would require more detailed examination involving the four-dimensional formalism usually applied to modulated structures. The final atom coordinates and equivalent isotropic displacement parameters for the subcell are given in Table 4 and selected interatomic distances in Table 5. A list of observed and calculated

TABLE 3. Crystallographic data and refinement parameters for rickturnerite.

General	
Temperature	293 K
Radiation, wavelength	Mo$K\alpha$, 0.71073 Å
Crystal system	Orthorhombic
Space group	*Pnma*
Unit-cell dimensions	$a = 5.8034(5)$, $b = 11.3574(9)$ $c = 12.9393(16)$ Å
Unit-cell volume	852.85(15) Å^3
Z	2
Calculated density	5.910 g cm^{-3}
Absorption coefficient	64.430 mm^{-1}
Crystal size (mm)	0.11 × 0.04 × 0.05
Data collection	
θ range	6.91–26.93º
h, k, l ranges	$-7 \rightarrow 7$, $-14 \rightarrow 12$, $-16 \rightarrow 16$
Total reflections collected	6061
Unique reflections (R_{int})	2058 (0.061)
Unique reflections $F > 4\sigma(F)$	1318
Structure refinement	
Refinement method	Full-matrix least-squares on F^2
No. of refined parameters, restraints	110, 1
Weighting coefficients a, b*	0.0488, 93.6534
Extinction coefficient	0.00000(7)
R_1 [$F > 4\sigma(F)$], wR_2 [$F > 4\sigma(F)$],	0.063, 0.132
R_1 all, wR_2 all	0.103, 0.152
Goodness-of-fit on F^2	1.028
Largest diff. peak and hole	5.92, −2.92 e Å^{-3}

Note: $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$;
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$;
$w = 1/[\sigma^2(F_o^2)+(aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$.

TABLE 4. Atomic coordinates and displacement parameters (Å) of atoms in rickturnerite.

Atom	Wyckoff position	Site occupation factor	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq} (Å^2)
Pb(1)	2*h*	1	½	0.7746(2)	0.60117(18)	0.0168(5)
Pb(2)	2*g*	1	0	0.7669(3)	0.1011(2)	0.0317(7)
Pb(3)	2*g*	1	0	0.7762(2)	0.8001(2)	0.0246(7)
Pb(4)	1*a*	1	0	0	0.6033(3)	0.0191(8)
Pb(5)	1*c*	1	½	0	0.8000(3)	0.0175(8)
Pb(6)	2*h*	1	½	0.7673(4)	0.2988(3)	0.0468(10)
Pb(7)	1*c*	1	½	0	0.1031(3)	0.0265(9)
Pb(8)	1*a*	1	0	0	0.2991(3)	0.0355(11)
Pb(9)	1*d*	0.8	½	½	1.0015(6)	0.0387(14)
Pb(10)	1*d*	0.1	½	½	1.072(3)	0.022(6)
Pb(11)	1*b*	0.78	0	½	0.4064(6)	0.0288(12)
Pb(12)	1*b*	0.22	0	½	0.4913(11)	0.02
Pb(13)	1*b*	0.1	0	½	1.007(2)	0.02
Cl(1)	2*g*	1	0	0.750(2)	0.4604(15)	0.049(6)
Cl(2)	2*h*	1	½	0.7498(14)	0.9618(12)	0.016(3)
Cl(3)	1*a*	1	0	0	0.9692(13)	0.012(4)
Cl(4)	1*c*	1	½	0	0.4624(16)	0.036(6)
Mg	2*f*	1	0.752(5)	½	0.700(3)	0.024(3)
O(1)	4*i*	1	0.743(7)	0.8756(14)	0.706(3)	0.018(4)
O(2)	4*i*	1	0.754(9)	0.8687(17)	0.201(4)	0.035(5)
OH(1)	2*g*	1	0	0.371(4)	0.670(4)	0.034(5)
OH(2)	2*h*	1	½	0.387(4)	0.718(4)	0.034(5)
OH(3)	2*f*	1	0.802(8)	½	0.848(3)	0.034(5)
OH(4)	2*f*	1	0.311(8)	½	0.528(3)	0.034(5)
OH(5)	2*h*	0.51	½	0.626(5)	0.179(4)	0.01
OH(6)	4*i*	0.25	0.782(14)	0.577(6)	0.210(8)	0.01

structure factors and anisotropic displacement parameters are available from www.minersoc.org/pages/e_journals/dep_mat.html.

X-ray powder diffraction data were obtained using a STOE STADI P diffractometer at the Department of Crystallography, St Petersburg State University, Russia. Data (in Å for Cu$K\alpha$) are given in Table 6. The data were refined to give $a = 5.82(1)$, $b = 22.80(3)$, $c = 25.88(2)$ Å, $V = 3432.0(5)$ Å^3.

The structure of rickturnerite contains 13 crystallographically independent Pb positions (Fig. 4). Of these, 5 sites are low-occupancy (Table 4). All the Pb–O bond lengths within a sphere of radius 3.6 Å were taken into consideration. The eight fully occupied Pb sites display four different types of coordination polyhedra. The Pb(1), Pb(3) and Pb(6) atoms each form three Pb–O bonds to two O atoms and one OH group, and three long bonds to Cl^- anions. The Pb(4), Pb(7), Pb(8) atoms, which are located in low-occupancy sites (Table 4) possess distorted square antiprism geometry. In one hemisphere they are coordinated by four O^{2-} anions, in the opposite hemisphere they are coordinated by four Cl^- anions. The coordination of the Pb(5) atom differs from the Pb(4), Pb(7) and Pb(8) atoms in the presence of only two long Pb–Cl bonds. The Pb(2) atom forms two short bonds to O^{2-} anions, two longer bonds to OH groups and three long bonds to Cl^- in another coordination sphere. The low-occupancy Pb sites are only coordinated by the oxygen atoms belonging to OH groups and Cl^- anions. All the Pb^{2+} coordination polyhedra are strongly distorted due to the stereoactivity of the s^2 lone-electron pairs on Pb^{2+} cations. There is one symmetrically independent Mg atom octahedrally coordinated by six OH groups (Fig. 5*a*).

The structure of rickturnerite seems to be best described in terms of both anion-centred and cation-centred coordination polyhedra. The O(1) and O(2) atoms form four short O–Pb bonds each, thus forming oxocentred [OPb_4] tetrahedra

TABLE 5. Selected interatomic distances (Å) for rickturnerite.

Pb(1)–O(1)	2.27(4)	Pb(8)–O(2)	2.42(5)
Pb(1)–O(1)	2.27(4)	Pb(8)–O(2)	2.42(5)
Pb(1)–OH(2)	2.38(5)	Pb(8)–O(2)	2.42(5)
Pb(1)–Cl(4)	3.127(12)	Pb(8)–O(2)	2.42(5)
Pb(1)–Cl(1)	3.438(10)		
Pb(1)–Cl(1)	3.438(10)	Pb(9)–OH(3)	2.65(5)
		Pb(9)–OH(3)	2.65(5)
Pb(2)–O(2)	2.24(5)	Pb(9)–OH(5)	2.71(5)
Pb(2)–O(2)	2.24(5)	Pb(9)–OH(5)	2.71(5)
Pb(2)–OH(6)	2.87(8)	Pb(9)–Cl(2)	2.883(16)
Pb(2)–OH(6)	2.87(8)	Pb(9)–Cl(2)	2.883(16)
Pb(2)–Cl(3)	3.150(10)		
Pb(2)–Cl(2)	3.422(8)	Pb(10)–OH(5)	1.99(6)
Pb(2)–Cl(2)	3.422(8)	Pb(10)–OH(5)	1.99(6)
		Pb(10)–OH(6)	2.57(9)
Pb(3)–O(1)	2.23(4)	Pb(10)–OH(6)	2.57(9)
Pb(3)–O(1)	2.23(4)	Pb(10)–OH(6)	2.57(9)
Pb(3)–OH(1)	2.38(5)	Pb(10)–OH(6)	2.57(9)
Pb(3)–Cl(3)	3.354(12)	Pb(10)–Cl(2)	3.17(2)
		Pb(10)–Cl(2)	3.17(2)
Pb(4)–O(1)	2.44(3)		
Pb(4)–O(1)	2.44(3)	Pb(11)–OH(4)	2.39(5)
Pb(4)–O(1)	2.44(3)	Pb(11)–OH(4)	2.39(5)
Pb(4)–O(1)	2.44(3)	Pb(11)–Cl(1)	2.93(2)
Pb(4)–Cl(1)	3.39(2)	Pb(11)–Cl(1)	2.93(2)
Pb(4)–Cl(1)	3.39(2)	Pb(11)–OH(6)	2.97(9)
Pb(4)–Cl(4)	3.427(11)	Pb(11)–OH(6)	2.97(9)
Pb(4)–Cl(4)	3.427(11)	Pb(11)–OH(6)	2.97(9)
		Pb(11)–OH(6)	2.97(9)
Pb(5)–O(1)	2.34(3)		
Pb(5)–O(1)	2.34(3)	Pb(12)–OH(4)	1.87(5)
Pb(5)–O(1)	2.34(3)	Pb(12)–OH(4)	1.87(5)
Pb(5)–O(1)	2.34(3)	Pb(12)–OH(1)	2.73(5)
		Pb(12)–OH(1)	2.73(5)
Pb(6)–OH(5)	2.23(5)	Pb(12)–Cl(1)	2.87(2)
Pb(6)–O(2)	2.26(5)	Pb(12)–Cl(1)	2.87(2)
Pb(6)–O(2)	2.26(5)		
Pb(6)–OH(6)	2.95(8)	Pb(13)–OH(3)	2.36(5)
Pb(6)–OH(6)	2.95(8)	Pb(13)–OH(3)	2.36(5)
Pb(6)–Cl(4)	3.386(14)	Pb(13)–OH(6)	3.04(10)
		Pb(13)–OH(6)	3.04(10)
Pb(7)–O(2)	2.45(5)	Pb(13)–OH(6)	3.04(10)
Pb(7)–O(2)	2.45(4)	Pb(13)–OH(6)	3.04(10)
Pb(7)–O(2)	2.45(4)		
Pb(7)–O(2)	2.45(4)	Mg–OH(3)	1.94(5)
Pb(7)–Cl(2)	3.379(16)	Mg–OH(2)	1.96(4)
Pb(7)–Cl(2)	3.379(16)	Mg–OH(2)	1.96(4)
Pb(7)–Cl(3)	3.380(9)	Mg–OH(1)	2.09(4)
Pb(7)–Cl(3)	3.380(9)	Mg–OH(1)	2.09(4)
		Mg–OH(4)	2.26(6)

(Fig. 5*a*). The O(1)Pb_4 and O(2)Pb_4 tetrahedra are linked by sharing Pb–Pb edges to form $[O_2Pb_3]^{2+}$ double chains, which extend along the *a* axis (Fig. 5*b*). Together with Cl^- ions, these chains form 2-dimensional blocks parallel to (100) (Fig. 6*a*). The $[O_2Pb_3]^{2+}$ chains are similar to

TABLE 6. X-ray powder diffraction data for rickturnerite, significant reflections are listed in bold.

I	d_{obs}	d_{calc}	*h*	*k*	*l*	*I*	d_{obs}	d_{calc}	*h*	*k*	*l*
1	8.542	8.536	2	0	2	4	1.799	1.8	4	3	3
1	8.094	8.064	3	0	1	1	1.787	1.787	13	1	4
100	**6.474**	6.47	4	0	0	1	1.784	1.784	1	2	10
23	6.37	6.222	4	0	1	1	1.773	1.772	2	2	10
7	5.717	5.691	3	0	3	2	1.77	1.77	8	1	10
44	**5.636**	5.622	0	1	1	3	1.762	1.762	13	0	6
16	4.315	4.32	4	1	0	3	1.759	1.76	6	3	1
20	4.287	4.287	2	0	5	3	1.75	1.751	3	2	10
6	4.04	4.038	4	1	2	2	1.744	1.744	6	3	2
3	3.981	4.01	1	1	4	6	1.738	1.739	13	1	5
2	3.828	3.825	5	0	4	6	1.729	1.729	11	1	8
2	3.323	3.322	7	0	3	12	1.722	1.722	7	1	11
28	**3.254**	3.268	4	0	6	17	1.69	1.689	3	3	6
73	**3.233**	3.22	1	0	7	**26**	**1.683**	1.682	14	1	4
13	3.183	3.194	5	1	4	10	1.673	1.673	0	1	13
31	**3.112**	3.111	8	0	2	7	1.663	1.661	0	3	7
2	3.067	3.08	2	1	6	6	1.606	1.606	14	0	7
1	3.066	3.056	5	0	6	4	1.602	1.601	16	0	2
18	2.968	2.973	8	0	3	8	1.599	1.597	14	1	6
57	**2.867**	2.868	7	0	5	4	1.591	1.592	5	1	13
10	2.84	2.84	0	0	8	5	1.585	1.585	0	2	12
12	2.816	2.816	1	1	7	3	1.577	1.577	13	2	4
25	**2.635**	2.635	8	0	5	2	1.574	1.574	2	2	12
6	2.565	2.565	9	0	4	5	1.569	1.569	13	1	8
3	2.293	2.291	8	0	7	1	1.561	1.561	7	3	6
2	2.211	2.211	5	2	5	1	1.487	1.487	2	2	13
1	2.2	2.197	3	0	10	4	1.484	1.481	11	3	2
9	2.168	2.17	4	2	6	6	1.482	1.48	11	2	9
12	2.159	2.16	8	2	0	2	1.382	1.382	12	1	12
17	2.152	2.152	9	0	7	3	1.363	1.362	7	1	15
12	2.142	2.143	4	0	10	3	1.361	1.36	10	3	8
8	2.129	2.13	9	1	6	3	1.359	1.359	8	2	13
14	2.118	2.118	7	2	4	6	1.357	1.357	11	3	7
2	2.104	2.104	5	2	6	6	1.355	1.355	18	1	4
3	2.026	2.035	11	1	4	2	1.295	1.295	16	2	7
4	2.019	2.019	8	2	4	1	1.294	1.294	7	4	5
2	2.014	2.014	12	1	1	1	1.207	1.207	11	4	4
1	1.954	1.953	12	1	3	1	1.205	1.205	15	2	11
1	1.88	1.879	13	0	4	2	1.203	1.203	9	4	7
2	1.8748	1.876	8	2	6	2	1.201	1.201	15	1	13
2	1.871	1.871	10	2	3	1	1.1989	1.199	19	0	9
2	1.867	1.867	7	2	7	2	1.197	1.197	15	3	7
2	1.862	1.862	3	3	2	1	1.195	1.195	17	3	1
1	1.852	1.853	4	3	0	2	1.185	1.184	3	0	19
1	1.821	1.821	11	2	1	2	1.181	1.182	17	3	3

those that are present in mendipite $Pb_3O_2Cl_2$ (Krivovichev and Burns, 2001*a*; Siidra *et al*., 2008*a*), chloroxiphite $[Pb_3O_2]CuCl_2(OH)_2$ (Siidra *et al*., 2008*b*), and damaraite $Pb_3O_2(OH)Cl$ (Krivovichev and Burns, 2001*a*). The $Mg(OH)_6$ octahedra share *trans*-edges to form $[Mg(OH)_4]^{2-}$ single chains running along the *a* axis, i.e. parallel to the chains of oxocentred $[OPb_4]$ tetrahedra (Fig. 5*c*). The $[Mg(OH)_4]^{2-}$ and $[O_2Pb_3]^{2+}$ chains are connected via Pb−OH bonds to form ordered layers parallel to the *ab* plane, which are designated in Figs 6*a* and 7 as *A* blocks.

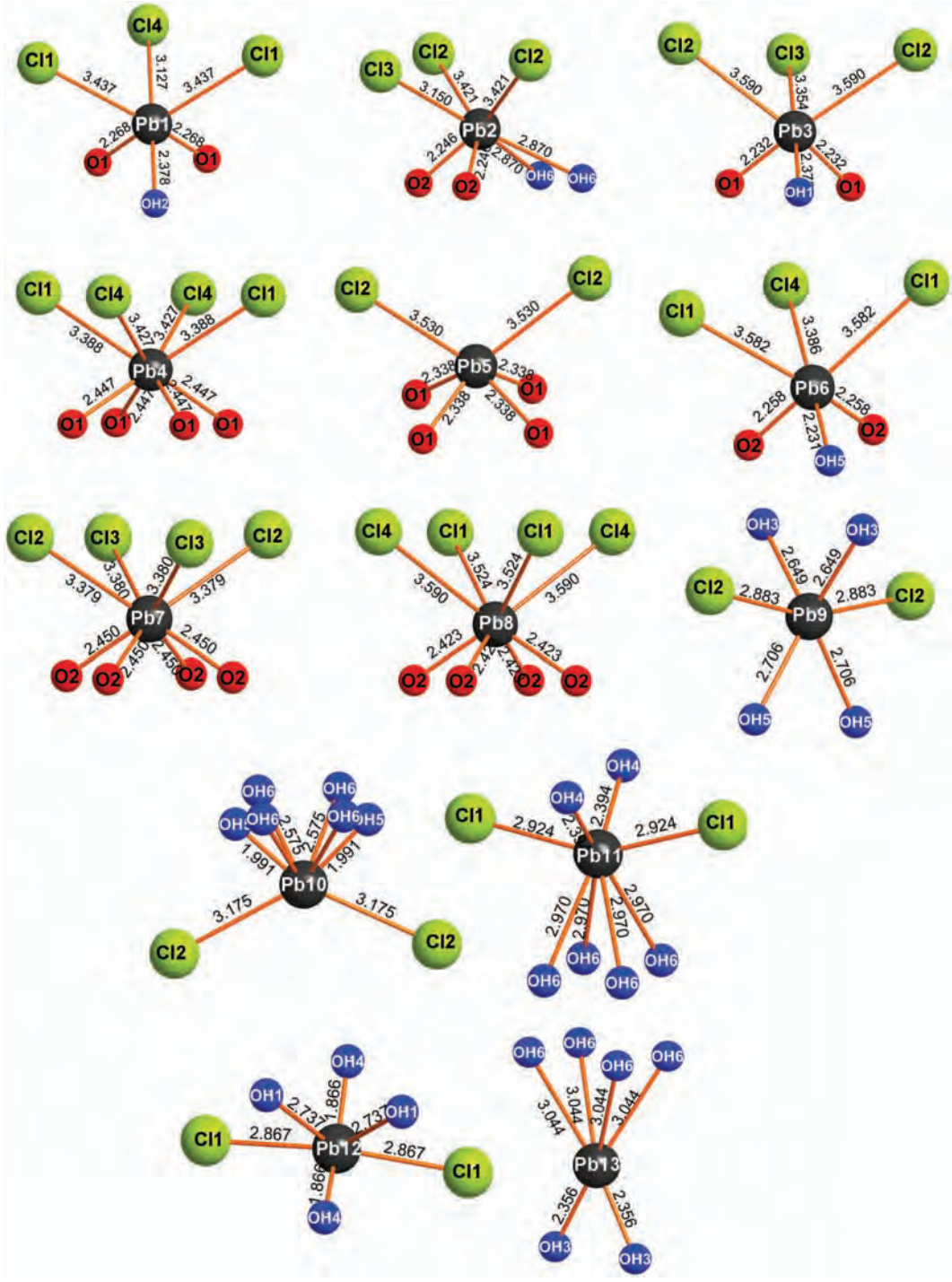


FIG. 4. The coordination of Pb^{2+} cations in the structure of rickturnerite. Note there are low site occupancy factors for Pb(9), Pb(10), Pb(11), Pb(12), Pb(13) and OH(5), OH(6) (see Table. 4).

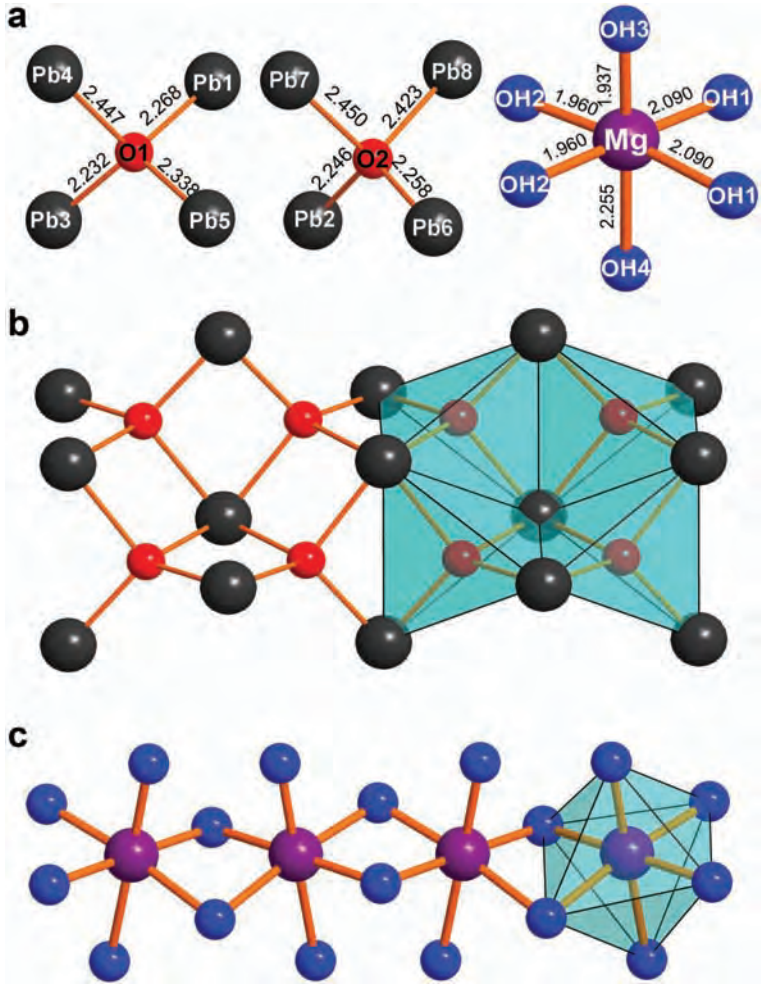
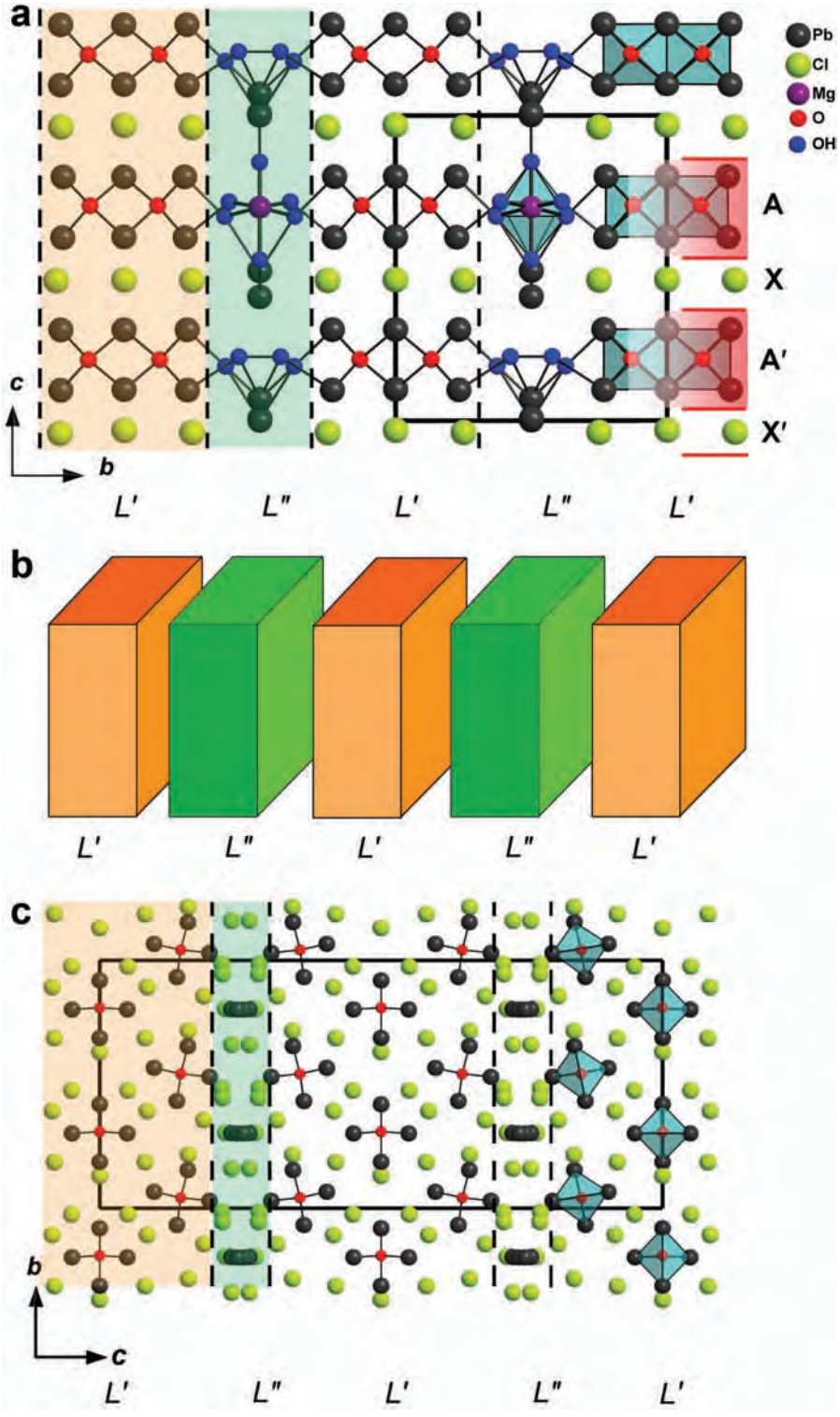


FIG. 5. Structural details of rickturnerite. (*a*) Coordination of the O(1) and O(2) atoms which form oxocentred OPb_4 tetrahedra, and of the Mg atom. (*b*) The structure of the $[O_2Pb_3]^{2+}$ chains. (*c*) The structure of the $[Mg(OH)_4]^{2-}$ chains.

Another layer, designated *A*′ (Fig. 6*a*), contains low-occupancy OH sites. The low-occupancy Pb sites are located within the chloride layers and designated in Figs 6*a* and 7 as *X* and *X*′. The structure of rickturnerite can thus be considered to contain a fully ordered part consisting of double

FIG. 6 (*facing page*). Structural details of rickturnerite (*a*) A projection of the crystal structure of rickturnerite along the *a* axis. The layer designated as A is formed by the sharing of oxocentred $[O_2Pb_3]^{2+}$ and cation centered $[Mg(OH)_4]^{2-}$ chains. The A′ layer contains OH sites with low site occupancy between the $[O_2Pb_3]^{2+}$ chains. The X and X′ layers are formed by chlorine and Pb sites with low occupancy. (*b*) The crystal structure of rickturnerite can be divided into two sets of blocks L′ (with completely occupied positions) and L (with low-occupancy sites). (*c*) A projection of the crystal structure of $Pb_{2+x}OCl_{2+2x}$ along the *a* axis with alternating L′ and L blocks. The L′ block contains fully occupied Cl sites and oxocentred $[O_2Pb_4]^{4+}$ chains. The L block contains low occupancy Pb sites and also Cl sites responsible for ionic conductivity.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Cl
Mg
O
OH
A
X
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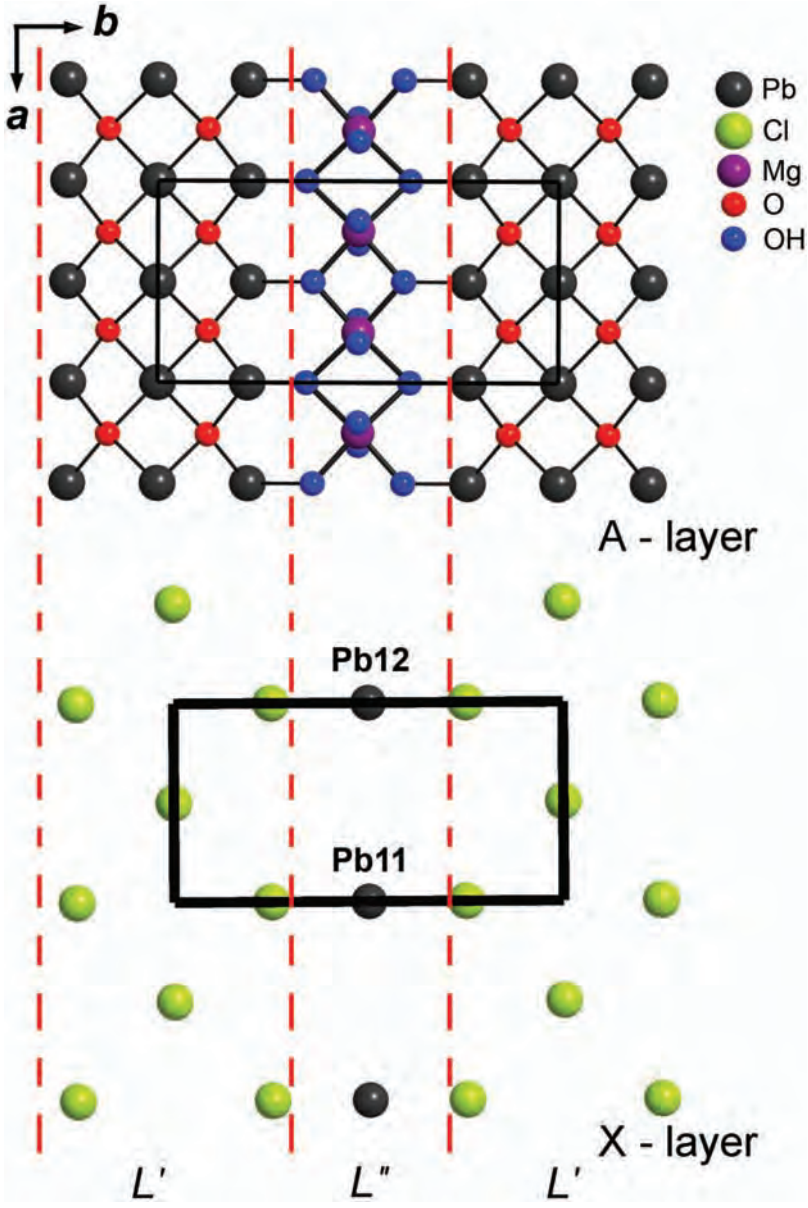

FIG. 7. A projection of the A- and X-layer in the crystal structure of rickturnerite. See the text for details.

$[O_2Pb_3]^{2+}$ chains and chlorine atoms (the *L′* blocks in Fig. 6*a*,*b*) with a disordered region designated as *L* between the ordered blocks and containing ordered $[Mg(OH)_4]^{2-}$ octahedral chains and low-occupancy Pb and OH sites. We suggest that ordering of these low-occupancy Pb sites is responsible for the weak supercell reflections.

The structure of rickturnerite is closely related to that of chloroxiphite $[Pb_3O_2]CuCl_2(OH)_2$ (Siidra *et al.*, 2008*b*). The $[Cu(OH)_2Cl_2]^{2-}$ chains in chloroxiphite are formed by face sharing of the $Cu(OH)_2Cl_2$ octahedra with apical chlorine atoms involved in connection between the layers.

Discussion and conclusion

Rickturnerite is a new Pb oxychloride mineral from Torr Works (Merehead) quarry in the UK. The mineral is structurally related to other Pb oxychlorides that contain different topological arrangements of linked [OPb_4] tetrahedra (Siidra *et al*., 2008*c*). Rickturnerite is most similar to the Pb-Cu oxychloride chloroxiphite, which has similar optical and physical properties. The $[O_2Pb_3]^{2+}$ double chains are widespread 1D units in the crystal structures of natural and synthetic Pb oxyhalides and other Pb oxysalts (Krivovichev *et al*., 2004) that contain 'additional' oxygen anions (anions that are not part of strong anionic complexes such as SO_4, PO_4, SiO_4, and VO_4). The arrangement of $[O_2Pb_3]^{2+}$ chains demonstrates some diversity in the structures of Pb oxyhalides (Fig. 8). These chains are in quincunx and shifted arrangement in the structures of $Pb_7O_4(OH)_4X_2$ (X = Cl, Br) (Siidra *et al*., 2008*d*; Krivovichev and Burns, 2001*b*) and chloroxiphite, respectively. The $[O_2Pb_3]^{2+}$ double chains can also have mutually perpendicular and zigzag arrangements as observed in mendipite and damaraite, respectively. As can be seen in Fig. 8*c*, the double chains are parallel in rickturnerite, which makes its structure different to that of chloroxiphite (Fig. 8*b*).

The subdivision of the structure of rickturnerite into the ordered (L') and disordered (L) blocks can be compared to the structure of the non-stoichiometric solid state ionic conductor $Pb_{2+x}OCl_{2+2x}$ (Siidra *et al*., 2007) (Fig. 6*c*). The structure of $Pb_{2+x}OCl_{2+2x}$ is based upon single $[O_2Pb_4]^{4+}$ chains of edge-sharing oxocentred tetrahedra and can be described as consisting of two-dimensional (2D) blocks L' and L. The L' block consists of ordered $[O_2Pb_4]^{4+}$ chains and Cl^- anions, whereas the L block contains closely spaced Pb and Cl sites with low occupancy.

Material from the Wesley mine (Alabaster, 1989) was also studied as part of this project and further rickturnerite specimens have been identified in the NHM collection as a result. This material is grey-white and contains no Cu, indicating that the slight green colour of the material at Torr Works (Merehead) quarry is almost certainly due to the trace Cu detected substituting for Mg. A very different specimen, possibly from Kombat mine, Namibia (although this remains unclear), has also shown traces of the new phase but more study is required to confirm the occurrence.

The origin of the manganese oxide pods and the lead oxychloride phases that they contain has been debated for many years (Green, 1958; Din *et al*., 1986). It is currently suggested (Turner, 2006)

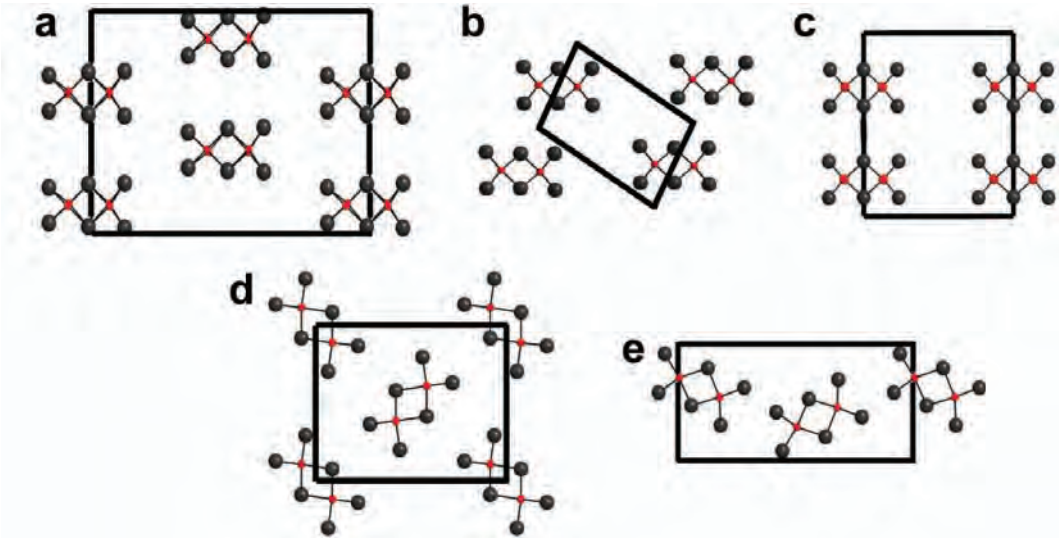

FIG. 8. The arrangement of $[O_2Pb_3]^{2+}$ chains in lead oxychloride minerals and inorganic compounds. (*a*) The quincunx arrangement in $Pb_7O_4(OH)_4X_2$ (X = Cl, Br). (*b*) Shifted $[O_2Pb_3]^{2+}$ chains in chloroxiphite. (*c*) The parallel arrangement in rickturnerite. (*d*) The mutually perpendicular arrangement in mendipite. (*e*) The zigzag arrangement in damaraite.

that all the Pb oxychlorides were formed when galena deposits emplaced into the Carboniferous limestones were locally exposed to the action of seawater. The subsequent oxidation of the galena initiated the deposition of manganate minerals, which adsorbed heavy metals from the sea water and the local environment. A later hydrothermal event heated the Pb-manganate deposits causing the galena to decompose, a variety of secondary minerals to form and the conversion of the manganates to manganese oxides. These oxides formed an impervious layer around the Pb-rich core, now charged with the other adsorbed heavy metals, and created a closed system. As temperatures fell and pH decreased, the assemblage of Pb oxychlorides found at Torr Works quarry formed within the closed system. It is likely that if a significant concentration of Mg is present within this microhabitat, the process includes the crystallization of rickturnerite, which appears to be one of the last Pb oxychlorides to form. It is significant to note however that rickturnerite has only been found in one such microhabitat at the locality to date, even though many of the manganese oxide pods contain significant Mg.

As the Torr Works (Merehead) specimens have only been found in recently collected material, their existence may indicate that the newer working areas at the quarry are intersecting manganese bearing veins or pods with different chemical signatures or formation conditions than have been previously encountered. This could signify further new species with future extensions of the quarry and is of considerable research interest.

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Cl2 Cl 0.5000 0.7498(14) 0.9618(12) 0.016(3) Uani 1 2 d S . .
Cl3 Cl 1.0000 1.0000 0.9692(13) 0.012(4) Uani 1 4 d S . .
Cl4 Cl 0.5000 1.0000 0.4624(16) 0.036(6) Uani 1 4 d S . .
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;
 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.
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